



# Kongeriget Danmark

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A handwritten signature in black ink, appearing to read 'Pia Petersen', is written over the date.  
Pia Petersen

21 MRS. 2003

**SUBTILASES****FIELD OF THE INVENTION**

The present invention relates to JP170 and BPN' like subtilases and to methods of construction such variants with altered properties, such as stability (e.g. thermostability or storage stability),  $\text{Ca}^{2+}$  dependency, pH dependent activity, improved performance in washing and cleaning applications.

**BACKGROUND OF THE INVENTION**

Enzymes have been used within the detergent industry as part of washing formulations for more than 30 years. Proteases are from a commercial perspective the most relevant enzyme in such formulations, but other enzymes including lipases, amylases, cellulases or mixtures of enzymes are also often used.

To improve the cost and/or the performance of proteases there is an ongoing search for proteases with altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered  $\text{Ca}^{2+}$  dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

The search for proteases with altered properties include both discovery of naturally occurring proteases, i.e. so called wild-type proteases but also alteration of well-known proteases by e.g. genetic manipulation of the nucleic acid sequence encoding said proteases. Knowledge of the relationship between the three-dimensional structure and the function of a protein has improved the ability to evaluate which areas of a protein to alter to affect a specific characteristic of the protein.

One family of proteases, which are often used in detergents, are the subtilases. This family has previously been further grouped into 6 different sub-groups by Siezen RJ and Leunissen JAM, 1997, Protein Science, 6, 501-523. One of these sub-groups is the Subtilisin family which includes subtilases such as BPN', subtilisin 309 (SAVINASE®, NOVOZYMES A/S), subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), subtilisin S41 (a subtilase from the psychrophilic Antarctic *Bacillus* TA41, Davail S et al. 1994, The Journal of Biological Chemistry, 269(26), 99. 17448-17453), subtilisin S39 (a subtilase from the psychrophilic Antarctic *Bacillus* TA39, Narinx E et al. 1997, Protein Engineering, 10 (11), pp. 1271-1279) and TY145 (a subtilase from *Bacillus* sp. TY145, NCIMB 40339 described in WO 92/17577).

However, despite the sequence homology between the subtilases belonging to the Subtilisin subgroup of subtilases, modelling of the three-dimensional structure of one subtilase

on the basis of the three-dimensional structure of another subtilase may result in an incorrect three-dimensional model structure because of structural differences.

5 Recently the three-dimensional structure of subtilase TY145 have been elucidated and it was found that there are several differences between this and the three-dimensional structure of BPN' also belonging to the Subtilisin subgroup of subtilases (Danish application PA 2003 00119).

10 The differences between the three-dimensional structures of TY145 and BPN' are confirmed by the three-dimensional structure of the subtilase "sphericase" from *Bacillus sphaericus* (PDB NO:1EA7, Protein Data Bank). The overall structure and many details of this subtilase are very homologous with the TY145 subtilase structure.

15 Now the inventors of the present invention disclose the three-dimensional structure of the subtilase JP170. This subtilase also has great structural differences compared to BPN' and TY145.

The subtilase JP170 and subtilases similar to JP170 are already known in the art, but the three-dimensional structure of the present invention has not been disclosed for such subtilases.

20 The JP170 subtilase was first described as protease A in WO 88/01293 to Novo Nordisk. Later the patent application WO 98/56927 to Novo Nordisk Biotech disclosed the amino acid (polypeptide) sequence of JP170 and the DNA sequence encoding JP170. The patents JP7-62152 and JP 4197182 to Lion Corp. disclosed the alkaline app. 46 kD protease Y produced by *Bacillus sp.* Y that is homologous to JP170 and the DNA sequence encoding protease Y. And in addition US 6,376,227 to Kao Corp. discloses physical characteristics as well as DNA and polypeptide sequences of alkaline proteases KP43, KP1790 and KP9860 which are also homologous to JP170. Recently variants of the KP43, KP9860, SD-521 and Y proteases among others were disclosed in EP 1209233. These variants have the accession numbers aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080. These proteases are highly homologous, and an alignment of KP43, KP9860, SD-521, Y and JP170 revealed at least 90% homology. Therefore JP170, Y (aay44619) and SD-521 (aam50084) represent these proteases in the alignments of the present application.

35 In the literature, modelling based on three-dimensional structures of proteins has been used to transfer advantageous properties from one protein to another. Miyazaki K et al.

2000, J Mol Biol, 297, pp.1015-1026 discloses enhancement of the thermostability and activity of the psychrophilic protease subtilisin S41 by methods of directed evolution.

Wintrode TL et al. 2000, Journal of Biological Chemistry, 275 (41), pp. 31635-31640 discloses conversion of a mesophilic subtilisin-like protease from *Bacillus sphaericus* SSII into its psychrophilic counterpart by methods of directed evolution. Wintrode et al. constructed the three-dimensional structural model of the SSII subtilase on basis of its homology with subtilisins Carlsberg, Savinase, BPN' and Thermitase, but according to the disclosure of the three-dimensional structure of the TY145 subtilase, the SSII subtilase pertain to the new group of TY145 like subtilases.

#### BRIEF DESCRIPTION OF THE INVENTION

The inventors have modified the amino acid sequence of a subtilase to obtain variants with improved properties, based on the three-dimensional structure of the subtilases JP170 and BPN'. The variants have altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered  $\text{Ca}^{2+}$  dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

Accordingly, the object of the present invention is to provide a method for constructing subtilases having altered properties, in particular to provide a method for constructing subtilases having altered properties as described above.

Thus, in its broadest aspect, the present invention relates to a method for constructing a variant of a parent subtilase, wherein the variant has at least one altered property as compared to said parent subtilase, which method comprises:

- i) analyzing the three-dimensional structure of the subtilase to identify, on the basis of an evaluation of structural considerations, at least one amino acid residue or at least one structural region of the subtilase, which is of relevance for altering said property;
- ii) constructing a variant of the subtilase, which as compared to the parent subtilase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property; and
- iii) testing the resulting subtilase variant for said property.

Although it has been described in the following that modification of the parent subtilase in certain regions and/or positions is expected to confer a particular effect to the thus produced subtilase variant, it should be noted that modification of the parent subtilase in any of such regions may also give rise to any other of the above-mentioned effects. For example,



any of the regions and/or positions mentioned as being of particular interest with respect to, e.g., improved thermostability, may also give rise to, e.g., higher activity at a lower pH, an altered pH optimum, or increased specific activity, such as increased peptidase activity.

Further aspects of the present invention relates to variants of a subtilase, the DNA encoding such variants and methods of preparing the variants. Still further aspects of the present invention relates to the use of the variants for various industrial purposes, in particular as an additive in detergent compositions. Other aspects of the present invention will be apparent from the below description as well as from the appended claims.

## 10 BRIEF DESCRIPTION OF FIGURES AND APPENDIX

Figure 1, Alignment of 3D sequences of protease JP170 (mature sequence from Appendix 1), SD-521 (aam50084 from EP 1209233) and protease Y (aay44619 from WO99/67370).

By 3D sequences is meant that the position of homologous residues are chosen by superposition of the 3D structures and subsequently the amino acid sequences are aligned based on these homologous positions.

Figure 2, Superposition of JP170 and Savinase 3D structures, with indication of calcium binding sites. JP170: light structure and three ion-binding sites. Savinase: dark structure and two ion-binding sites.

Figure 3, Matrix of homology between subtilases pertaining to the JP170 and BPN' subgroups. The sequences are identified by sequence database accession numbers.

APPENDIX 1 shows the structural coordinates for the solved crystal structure of JP170.

## 25 DEFINITIONS

Prior to discussing this invention in further detail, the following terms and conventions will first be defined.

For a detailed description of the nomenclature of amino acids and nucleic acids, we refer to WO 00/71691 page 5, hereby incorporated by reference. A description of the nomenclature of modifications introduced in a polypeptide by genetic manipulation can be found in WO 00/71691 page 7-12, hereby incorporated by reference.

The term "subtilases" refer to a sub-group of serine protease according to Siezen *et al.*, *Protein Engng.* 4 (1991) 719-737 and Siezen *et al.* *Protein Science* 6 (1997) 501-523. Ser-

ine proteases or serine peptidases is a subgroup of proteases characterised by having a serine in the active site, which forms a covalent adduct with the substrate. Further the subtilases (and the serine proteases) are characterised by having two active site amino acid residues apart from the serine, namely a histidine and an aspartic acid residue.

5 Subtilases are defined by homology analysis of more than 170 amino acid sequences of serine proteases previously referred to as subtilisin-like proteases. The subtilases may be divided into 6 sub-divisions, i.e. the Subtilisin family, the Thermitase family, the Proteinase K family, the Lantibiotic peptidase family, the Kexin family and the Pyrolysin family.

The Subtilisin family (EC 3.4.21.62) may be further divided into 3 sub-groups, i.e. I-S1  
10 ("true" subtilisins), I-S2 (highly alkaline proteases) and intracellular subtilisins. Definitions or grouping of enzymes may vary or change, however, in the context of the present invention the above division of subtilases into sub-division or sub-groups shall be understood as those described by Siezen et al., *Protein Engng.* 4 (1991) 719-737 and Siezen et al. *Protein Science* 6 (1997) 501-523.

15

The term "parent" is in the context of the present invention to be understood as a protein, which is modified to create a protein variant. The parent protein may be a naturally occurring (wild-type) polypeptide or it may be a variant thereof prepared by any suitable means. For instance, the parent protein may be a variant of a naturally occurring protein which has  
20 been modified by substitution, chemical modification, deletion or truncation of one or more amino acid residues, or by addition or insertion of one or more amino acid residues to the amino acid sequence, of a naturally-occurring polypeptide. Thus the term "parent subtilase" refers to a subtilase which is modified to create a subtilase variant.

25 The term "variant" is in the context of the present invention to be understood as a protein which has been modified as compared to a parent protein at one or more amino acid residues.

The term "modification(s)" or "modified" is in the context of the present invention to be understood as to include chemical modification of a protein as well as genetic manipulation of  
30 the DNA encoding a protein. The modification(s) may be replacement(s) of the amino acid side chain(s), substitution(s), deletion(s) and/or insertions in or at the amino acid(s) of interest. Thus the term "modified protein", e.g. "modified subtilase", is to be understood as a protein which contains modification(s) compared to a parent protein, e.g. subtilase.

35

The term "JP170 subtilase" or "JP170 like subtilase" should in the context of the present invention be understood as a subtilase belonging to the Subtilisin group according to Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 58% homology to JP170 SEQ ID NO:1. Thus, among others the alkaline proteases KP43, KP1790, KP9860, Y and SD-521 are subtilases belonging to the JP170 subgroup of subtilases. In the context of the present invention a JP170 subtilase has three ion-binding sites. However, the number of ion-binding sites may vary in similar structures depending on the medium used for crystallisation. It appears e.g. that two of five ion-binding sites of *Bacillus sphaericus* "sphericase" (PDB NO:1EA7, Protein Data Bank) were due to a calcium containing crystallisation medium.

The term "(a) BPN' subtilase" or "(a) BPN' like subtilase" should in the context of the present invention be understood as a subtilase belonging to the Subtilisin group according to Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 61% homology to BPN' SEQ ID NO:5. Such a BPN' like subtilase is for example Savinase. In the context of the present invention a BPN' subtilase has two ion-binding sites. A BPN' like subtilase may, in the context of the present invention, belong to branch I-S of the subtilisins i.e. to branch I-S1, the "true" subtilisins or I-S2, the highly alkaline proteases (Siezen et al., *Protein Engng.* 4 (1991) 719-737).

"Homology" or "homologous to" is in the context of the present invention to be understood in its conventional meaning and the "homology" between two amino acid sequences should be determined by use of the "Similarity" defined by the GAP program from the University of Wisconsin Genetics Computer Group (UWGCG) package using default settings for alignment parameters, comparison matrix, gap and gap extension penalties. Default values for GAP penalties, i.e. GAP creation penalty of 3.0 and GAP extension penalty of 0.1 (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711). The method is also described in S.B. Needleman and C.D. Wunsch, *Journal of Molecular Biology*, 48, 443-445 (1970). Identities can be extracted from the same calculation. The homology between two amino acid sequences can also be determined by "identity" or "similarity" using the GAP routine of the UWGCG package version 9.1 with default setting for alignment parameters, comparison matrix, gap and gap extension penalties can also be applied using the following parameters: gap creation penalty = 8 and gap extension penalty = 8 and all other parameters kept at their default values. The output from the routine is besides the amino acid alignment the

calculation of the "Percent Identity" and the "Similarity" between the two sequences. The numbers calculated using UWGCG package version 9.1 is slightly different from the version 8.

- 5 The term "position" is in the context of the present invention to be understood as the number of an amino acid in a peptide or polypeptide when counting from the N-terminal end of said peptide/polypeptide. The position numbers used in the present invention refer to different subtilases depending on which subgroup the subtilase belongs to.
- 10 As mentioned above the alkaline subtilases KP43, KP1790, KP9860, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233 belong to the JP170 subgroup, based on sequence homology. Due to the extensive homology only subtilase Y and SD-521 are aligned with JP170. The Y subtilase and SD-521 subtilase are numbered according to SEQ ID NO:2 and 3 respectively.
- 15 Likewise other subtilases belonging to the JP170 subgroup are numbered individually according to their own sequence. However in order to determine homologous positions in such other subtilases an alignment with the each of SEQ ID's NO:1, 2 and 3 is conducted according to the GAP procedure described above. Subsequently the homologous positions
- 20 are determined with reference to the most homologous of SEQ ID's NO:1, 2 and 3.

Alternatively subtilases belonging to the JP170 subgroup can be numbered by reference to the positions of JP170 subtilase (SEQ ID NO:1).

- 25 Subtilases belonging to the BPN' subgroup refers to the positions of Subtilisin Novo (BPN') from *B. amyloliquefaciens*.

#### DETAILED DESCRIPTION OF THE INVENTION

- Despite the great homology of the subtilases described above the inventors of the present invention have elucidated the three-dimensional structure of JP170, SEQ ID NO:1 by X-ray crystallography and found that there are several differences between this and the three-dimensional structure of BPN'. The inventors of the present invention have further compared the sequence homology of subtilases belonging to the Subtilisin subgroup. This is shown in Figure 3 of the present invention.
- 30

On the basis of this comparison the inventors of the present invention suggest to divide the Subtilisin subgroup so that the JP170 subtilases become a separate subgroup in addition to the subgroups of BPN' subtilases and TY145 subtilases (DKPTO, PA 2003 00119).

5 JP170 subtilases

As described above a JP170 like subtilase is in the context of the present invention to be understood as a subtilase which has at least 58% homology to SEQ ID NO:1. In particular said JP170 subtilase may have at least 60% homology to SEQ ID NO:1, such as at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at  
10 least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to JP170, i.e. to SEQ ID NO:1.

In a first embodiment of the present invention a JP170 subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of  
15 JP170, i.e. it may be homologous to the three-dimensional structure defined by the structure coordinates in Appendix 1.

As it is well-known to a person skilled in the art that a set of structure coordinates for a protein or a portion thereof is a relative set of points that define a shape in three dimensions, it is possible that an entirely different set of coordinates could define an identical or a similar  
20 shape. Moreover, slight variations in the individual coordinates may have little or no effect on the overall shape.

These variations in coordinates may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates of JP170 (Appendix 1) may be manipulated by crystallographic permutations of the structure coordinates, fraction-  
25 alization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, said variations may be due to differences in the primary amino acid sequence.

If such variations are within an acceptable standard error as compared to the structure coordinates of Appendix 1 said three-dimensional structure is within the context of the present  
30 invention to be understood as being homologous to the structure of Appendix 1. The standard error may typically be measured as the root mean square deviation of e.g. conserved backbone residues, where the term "root mean square deviation" (RMS) means the square root of the arithmetic mean of the squares of the deviations from the mean.



As it is also well-known to a person skilled in the art that within a group of proteins which have a homologous structure there may be variations in the three-dimensional structure in certain areas or domains of the structure, e.g. loops, which are not or at least only of a small importance to the functional domains of the structure, but which may result in a big root mean square deviation of the conserved residue backbone atoms between said structures.

Thus it is well known that a set of structure coordinates is unique to the crystallised protein. No other three dimensional structure will have the exact same set of coordinates, be it a homologous structure or even the same protein crystallised in different manner. There are natural fluctuations in the coordinates. The overall structure and the inter-atomic relationship can be found to be similar. The similarity can be discussed in terms of root mean square deviation of each atom of a structure from each "homologous" atom of another structure. However, only identical proteins have the exact same number of atoms. Therefore, proteins having a similarity below 100% will normally have a different number of atoms, and thus the root mean square deviation can not be calculated on all atoms, but only the ones that are considered "homologous". A precise description of the similarity based on the coordinates is thus difficult to describe and difficult to compute for homologous proteins. Regarding the present invention, similarities in 3D structure of different subtilases can be described by the content of homologous structural elements, and/or the similarity in amino acid or DNA sequence. For sequences having no deletions or insertions a RMS for the calcium atoms can be calculated.

Examples of JP170 like subtilases include the alkaline proteases KP43, KP1790, KP9860, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233, however to the best of our knowledge the three-dimensional structure has not been solved for any of these subtilases.

Accordingly, a preferred embodiment of the present invention is a parent subtilase or a subtilase variant which is at least 58% homologous to the sequence of SEQ ID NO:1, preferably at least 60, at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homologous to the sequence of SEQ ID NO:1, and optionally said subtilase further comprises the following structural characteristics:

- a) a twisted beta-sheet with 7 strands,
- b) six alpha helices,
- c) three ion-binding sites and

not comprising the Strong and Weak ion-binding site of the BPN' like subtilases, and with  
 5 the exception of the subtilases JP170, KP1790, KP9860, KP43, Y, SD-521 and variants  
 aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081,  
 aam50080 of EP 1209233.

The JP170 subtilase of the present invention is encoded by an isolated nucleic acid se-  
 10 quence, which nucleic acid sequence encodes a subtilase which has at least 58% homol-  
 ogy to SEQ ID NO:1. In particular said nucleic acid sequence encodes a subtilase that has  
 at least 60% homology to SEQ ID NO:1, such as at least 65%, at least 70%, at least 75%,  
 at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least  
 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to  
 15 SEQ ID NO:1, i.e. to the amino acid sequence of JP170.

Further the isolated nucleic acid sequence encoding a JP170 subtilase of the invention hy-  
 bridizes with a complementary strand of a nucleic acid sequence encoding the amino acid  
 sequence of SEQ ID NO:1 preferably under low stringency conditions, at least under me-  
 20 dium stringency conditions, at least under medium/high stringency conditions, at least un-  
 der high stringency conditions, at least under very high stringency conditions.

Suitable experimental conditions for determining hybridization at low, medium, or high  
 stringency conditions between a nucleotide probe and a homologous DNA or RNA se-  
 25 quence involves presoaking of the filter containing the DNA fragments or RNA to hybridize  
 in 5 x SSC (Sodium chloride/Sodium citrate, Sambrook et al. 1989) for 10 min, and prehy-  
 bridization of the filter in a solution of 5 x SSC, 5 x Denhardt's solution (Sambrook et al.  
 1989), 0.5 % SDS and 100 µg/ml of denatured sonicated salmon sperm DNA (Sambrook et  
 al. 1989), followed by hybridization in the same solution containing a concentration of  
 30 10ng/ml of a random-primed (Feinberg, A. P. and Vogelstein, B. (1983) *Anal. Biochem.*  
 132:6-13), <sup>32</sup>P-dCTP-labeled (specific activity > 1 x 10<sup>9</sup> cpm/µg ) probe for 12 hours at ca.  
 45°C. The filter is then washed twice for 30 minutes in 2 x SSC, 0.5 % SDS at least \* 55°C  
 (low stringency), more preferably at least 60°C (medium stringency), still more preferably at  
 least 65°C (medium/high stringency), even more preferably at least 70°C (high stringency),  
 35 and even more preferably at least 75°C (very high stringency).

BPN' subtilases

As described above a BPN' subtilase is in the context of the present invention to be understood as a subtilase which has at least 61% homology to SEQ ID NO:4. In particular said BPN' subtilase may have at least 65%, such as at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to BPN', i.e. to SEQ ID NO:4.

In one embodiment of the present invention a BPN' subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of BPN' as defined by the structure coordinates given in PDB Nos. 1SBT and 1GNS (Protein Data Bank), or one of the several other structures of BPN' that are accessible from the Protein Data Bank. Variations between homologous structures may occur for several reasons as described above. Thus a BPN' subtilase within the context of the present invention is to be understood as any subtilase having the structural characteristics pertaining to the BPN' subtilases as described above, and in addition such subtilases does preferably not have further structural characteristics which are not present in the BPN' subtilases as described herein. Further a BPN' subtilase of the present invention may have the necessary percentage of similarity with SEQ ID NO:4.

Examples of BPN' like subtilases include the subtilisin 309 (PDB NO:1SVN, SAVINASE®, NOVOZYMES A/S) and subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), among others.

In figure 1 of R.J. Siezen and J.A.M Leunissen (Protein science, Vol. 6 (3), pp. 501-523, 1997) page 502 a structure of subtilases is described. A subtilase consists of 6-8 helices, 11 strands of which 7 are central in a twisted beta-sheet. Two ion-binding sites are mentioned, the so called "Strong" and "Weak" calcium-binding sites. It was later discovered that for some structures (subtilisin DY PDB no. 1BH6, 1998), the Weak calcium-binding site was shown to be a Na (sodium) binding site when the calcium concentration in the crystallization medium was low. Thus, in the following we refer to ion-binding sites instead of calcium-binding sites.

The BPN' subtilase of the present invention is encoded by an isolated nucleic acid sequence, which nucleic acid sequence encodes a subtilase which has at least 61% homology to SEQ ID NO:4. In particular said BPN' subtilase may have at least 65%, such as at

least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to BPN', i.e. to SEQ ID NO:4.

- 5 Further the isolated nucleic acid sequence encoding a BPN' subtilase of the invention hybridizes with a complementary strand of the nucleic acid sequence encoding the amino acid sequence of SEQ ID NO:4 preferably under low stringency conditions, at least under medium stringency conditions, at least under medium/high stringency conditions, at least under high stringency conditions, at least under very high stringency conditions.

10

### **Three-dimensional structure of JP170 subtilases**

The JP170 subtilase was used to elucidate the three-dimensional structure forming the basis for the present invention.

- 15 The structure of JP170 was solved in accordance with the principle for x-ray crystallographic methods, for example, as given in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989.

- 20 The structural coordinates for the solved crystal structure of JP170 are given in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT) as set forth in Appendix 1. It is to be understood that Appendix 1 forms part of the present application. In the context of Appendix 1, the following abbreviations are used: CA refers to c-alpha (carbon atoms) or to calcium ions, (however to avoid misunderstandings we use the full names "c-alpha atoms" and "calcium" or "ion" in the present specification). Amino acid residues are given in their standard three-letter code. The attached structural coordinates
- 25 contain the protease structure, and an inhibitor structure Cl2 as well as water molecules. The protease coordinates has a chain identification called A, whereas the Cl2 inhibitor is called B, the calcium ions are called C, and the water is W. In the following the positions of the mentioned residues refer to the sequence of JP170 as disclosed in SEQ ID NO:1.

- 30 The JP170 structure consists of two domains, a catalytic domain and a C-terminal domain. The structure of the catalytic domain shows the same overall fold as found in the S8 family of subtilisins. The structure comprises a twisted beta-sheet with 7 strands arranged in the following sequential order S2, S3, S1, S4, S5, S6, S7.

There are six alpha helices in the catalytic domain structure of which number H1 contains residues 9-17, H2 contains residues 68-76, H3 contains residues 110-119, H4 contains residues 139-150, H5 contains residues 253-273 and H6 contains residues 281-291.

The C-terminal domain comprises a strand motif, a so called "beta sandwich" consisting of sheets a and b. The sheet in this domain is combined of strands in an anti-parallel fashion, whereas the strand in the catalytic domain is combined in parallel. The sequential order of the strands can be denoted as: S1a-S1b-S3a-S3b-S4b-S4a-S2b-S2a with the beta sandwich organised as to the two sheets S1a, S3a, S4a, S2a and S1b, S3b, S4b, S2b.

The JP170 subtilases are shown to lack the well-known Strong and Weak ion-binding sites of the BPN' subtilases. However, the JP170 subtilases have three ion-binding sites which are not present in the BPN' subtilisin structures. This can be seen in the structural alignment presented in Figure 2. These three ion-binding sites are hereinafter referred to as Site 1, which is placed in the catalytic domain, and Site 2 and 3 which are placed in the non-catalytic C-terminal domain.

Thus in relation to the atomic coordinates disclosed in Appendix 1, the ion-binding sites of JP170 are located at:

Site 1 - calcium atom named A601 CA

Site 2 - calcium atom named A603 CA, and

Site 3 - calcium atom named A602 CA in the PDB table (Appendix 1).

The position of an ion-binding site can be defined by the distance to four specific atoms in the core structure. The distance from the ion-binding site to the c-alpha atoms of the three active site residues has been chosen. Throughout the subtilases the residues Ser, His and Asp in the active site are highly conserved. In JP170 they are Asp30, His68 and Ser254. The fourth distance chosen is the distance to the c-alpha atom of the amino acid residue coming first after the active site serine residue in the sequence (herein after called "next to Ser"); in the 3D structure of JP170 it is Met255.

In a preferred embodiment of the present invention, the distance between:

- a) ion-binding site 1 and i) Asp c-alpha atom is 26.70-28.70Å, ii) His c-alpha atom is 22.10-24.10Å, iii) Ser c-alpha atom is 16.95-18.95Å, iv) next to Ser c-alpha atom is 15.30-17.30Å,
- b) ion-binding site 2 and i) Asp c-alpha atom is 33.50-35.50Å, ii) His c-alpha atom is 37-39Å, iii) Ser c-alpha atom is 29.40-31.40Å, iv) next to Ser c-alpha atom is 30.70-



32.70Å,

- c) ion-binding site 3 and i) Asp c-alpha atom is 41.50-43.50Å, ii) His c-alpha atom is 42.90-44.90Å, iii) Ser c-alpha atom is 34.50-36.50Å, iv) next to Ser c-alpha atom is 35-37Å.

5

Below are the specific distances between the four chosen c-alpha atoms and the three ion binding sites of the JP170 subtilase given in Å:

	site 1	site 2	site 3
Met255	16.34	31.68	36.02
10 His68	23.12	38.03	43.87
Asp30	27.69	34.49	42.48
Ser254	17.95	30.41	35.51
site 1	0	35.29	32.92
site 2	35.29	0	14.08
15 site 3	32.92	14.08	0

However these distances may vary from one subtilase to the other. The present distances are given with a calcium ion in the structure. If a sodium ion was bound instead the distances would be shifted a little bit. Generally the distances can vary  $\pm 0.80\text{Å}$ , preferably  $\pm 0.70\text{Å}$ ,  $\pm 0.60\text{Å}$ ,  $\pm 0.50\text{Å}$ ,  $\pm 0.40\text{Å}$ , or most preferably  $\pm 0.30\text{Å}$ .

Further, in the JP170 like subtilases, the peptide structure circumventing ion-binding site 1 up to a distance of 10 Å is composed of the amino acid residues placed in positions 183-189, 191-204 and 224-225.

25 The peptide structure circumventing ion-binding site 2 up to a distance of 10 Å is composed of residues 378-393.

The peptide structure circumventing ion-binding site 3 up to a distance of 10 Å is composed of residues 348, 350, 352, 363-370, 380-383, 391-400 and 414-420.

30 In comparison with the BPN' like subtilase structures the structure of the JP170 like subtilases can be divided into a "core subtilase-like" region, an "intermediate" region and a "nonhomologous" region.

The active site can be found in the core subtilase-like region, which is structurally closely related to the BPN' structures. The core subtilase-like region is composed of residues 17-34, 197-209 and 216-232, and contains the alpha-helix H3 and the central alpha-helix H5 in

which the active site serine residue is situated in the N-terminal part. The core subtilase-like region has an RMS lower than 1.2.

Outside the core subtilase-like region the structure of the JP170 like subtilase differs from the BPN' structures to a greater extent.

5

The intermediate region consists of residues 42-46, 150-186, 245-272 and 278-296. The intermediate region has an RMS bigger than 1.2 and less than 1.8. The relationships between the three-dimensional structure and functionality are potentially difficult to predict in this region of the JP170 like subtilases.

10

The nonhomologous region consists of residues 1-16, 35-41, 47-149, 187-196, 210-215, 233-244, 273-277 and 297-316. The nonhomologous region has a RMS higher than 1.8.

The relationships between the three-dimensional structure and functionality are very difficult to predict in this region of the JP170 like subtilases.

15

Many loops in the 3D structure of the JP170 like subtilases differ significantly from the BPN' type structures, both in length and in content of amino acid residues. The following loops or protein sequence stretches of JP170 are compared to Savinase (in parenthesis):

G32-H43 (G34-H39)

20 E44-Y54 (P40-A48)

G57-G67 (V51-G63)

N79-N82 (I75-V81)

I96-P107 (V95-S105)

A108-S119 (106-N117)

25 A131-Y137 (S128-S132)

T138-D152 (A133-G146)

E162-I169 (S156-I165)

G173-T180 (A169-A176)

E185-N199 (D181-N184)

30 G208-D218 (G193-D197)

S232-K246 (G211-T213)

D294-N303 (S256-L262)

The loops N79-N82 (I75-V81) and G208-D218 (G193-D197) are in contact with a ion-binding site in Savinase, but not in JP170. Similarly the loop E185-N199 (D181-N184) is in

35

contact with a ion-binding site in JP170, but not in Savinase. This knowledge opens for possibilities of adding or removing ion-binding sites to subtilases of the JP170 and BPN' like types.

- 5 A good example of the difference is the loop S232-K246 which has 15 residues compared to the corresponding BPN' type loop G211-T213 (in Savinase), which has only three residues. In the JP170 like subtilases, the loop folds back to the substrate binding site, especially the P' parts of the substrate binding site. The loop is situated close to the substrate as illustrated by the Cl2 inhibitor bound in the 3D structure attached (Appendix 1).

10

The location of loop S232-K246 can be described in relation to the four specific residues as described above. The distance from the CA atom of residue W240 in the loop to the CA atoms of the active site residues are:

Residue	H68	D30	S254	M255
Distance, Å	11.45	18.51	13.06	11.94

- 15 As mentioned above, distances like these can vary  $\pm 0.80\text{\AA}$ , preferably  $\pm 0.70\text{\AA}$ ,  $\pm 0.60\text{\AA}$ ,  $\pm 0.50\text{\AA}$ ,  $\pm 0.40\text{\AA}$ , or most preferably  $\pm 0.30\text{\AA}$ .

Furthermore, distances from the residues of JP170 loop S232-K246 to atoms of the Cl2 inhibitor can be calculated. These distances are:

- 20 from CA atom of W240 to CA atom of R62 in Cl2 is  $7.49\text{\AA}$ ,  
 from CA atom of F239 to CA atom of R62 in Cl2 is  $8.39\text{\AA}$ ,  
 from CA atom of S238 to CA atom of R62 in Cl2 is  $8.42\text{\AA}$ ,  
 from CA atom of S237 to CA atom of R62 in Cl2 is  $9.44\text{\AA}$ ,  
 from CA atom of S238 to CA atom of E60 in Cl2 is  $9.42\text{\AA}$ .

25

The distances from JP170 active site residue S254 to atoms of the Cl2 inhibitor, as placed in the 3D coordinates of Appendix 1, are:

- from CA atom of S254 to CA atom of E60 in Cl2 is  $5.25\text{\AA}$ ,  
 from CA atom of S254 to CA atom of R62 in Cl2 is  $11.55\text{\AA}$ ,  
 30 from CA atom of S254 to CA atom of T58 in Cl2 is  $7.06\text{\AA}$ ,  
 from CA atom of S254 to CA atom of M59 in Cl2 is  $4.71\text{\AA}$ .

The distances can vary  $\pm 0.80\text{\AA}$ , preferably  $\pm 0.70\text{\AA}$ ,  $\pm 0.60\text{\AA}$ ,  $\pm 0.50\text{\AA}$ ,  $\pm 0.40\text{\AA}$ , or most preferably  $\pm 0.30\text{\AA}$ .

A preferred JP170 like subtilase variant has a deletion in the region S232-K246, and the subsequent insertion of one or more residues to partly or completely remove the loop. Preferred variants comprises the deletion of L233-S245 + insertion of Asn, deletion of L233-D244 + insertion of Gly or deletion of S232-D244 + insertion of Gly.

5

#### **Homology building of JP170 and BPN' subtilases**

A model structure of a JP170 like subtilase or a BPN' like subtilase can be built using the Homology program or a comparable program, e.g., Modeller (both from Molecular Simulations, Inc., San Diego, CA). The principle is to align the amino acid sequence of a protein for which the 3D structure is known with the amino acid sequence of a protein for which a model 3D structure has to be constructed. The structurally conserved regions can then be built on the basis of consensus sequences. In areas lacking homology, loop structures can be inserted, or sequences can be deleted with subsequent bonding of the necessary residues using, e.g., the program Homology. Subsequent relaxing and optimization of the structure should be done using either Homology or another molecular simulation program, e.g., CHARMM from Molecular Simulations.

#### **Methods for designing JP170 and BPN' subtilase variants**

Comparisons of the molecular dynamics of different proteins can give a hint as to which domains are important or connected to certain properties pertained by each protein.

The present invention comprises a method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

- a) modelling the parent JP170 subtilase on the three-dimensional structure of a JP170 subtilase to produce a three-dimensional structure of the parent JP170 subtilase;
- b) identifying on the basis of the comparison in step a) at least one structural part of the parent JP170 subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- c) modifying the nucleic acid sequence encoding the parent JP170 subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
- d) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 subtilase;
- e) isolating the produced subtilase;

- f) purifying the isolated subtilase and
- g) recovering the purified subtilase.

Further the present invention comprises a method of producing a variant of a parent Subtilisin family subtilase, such as a BPN' like subtilase, the variant having at least one altered property as compared to the parent Subtilisin family subtilase, the method comprising:

- a) modelling the parent Subtilisin family subtilase on the three-dimensional structure of a Subtilisin family subtilase to produce a three-dimensional structure of the parent Subtilisin family subtilase;
- 10 b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a JP170 like subtilase;
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent Subtilisin family subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- 15 d) modifying the nucleic acid sequence encoding the parent Subtilisin family subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
- e) expressing the modified nucleic acid sequence in a host cell to produce the variant
- 20 Subtilisin family subtilase,
- f) isolating the produced subtilase,
- g) purifying the isolated subtilase and
- h) recovering the purified subtilase.

25 Further the present invention comprises a method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

- a) modelling the parent JP170 like subtilase on the three-dimensional structure of a JP170 like subtilase to produce a three-dimensional structure of the parent JP170 like
- 30 subtilase;
- b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a Subtilisin family subtilase;
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent JP170 like subtilase, wherein an alteration in said structural part is predicted to
- 35 result in an altered property;



- d) modifying the nucleic acid sequence encoding the parent JP170 like subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
- 5 e) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 like subtilase;
- f) isolating the produced subtilase;
- g) purifying the isolated subtilase and
- h) recovering the purified subtilase.

10

### Stability - alteration of ion-binding sites

As described above the JP170 subtilases has three new ion-binding sites not present in the BPN' subtilisin structures but lacks the Strong and Weak ion-binding site of the BPN' subtilases. Stability of the ion-binding site is of crucial importance for the functionality of the enzyme. Therefore alterations of the ion-binding sites are likely to result in alterations of the stability of the enzyme.

15

### Improved stability

Stabilisation of a JP170 subtilase may possibly be obtained by alterations in the positions close to the ion-binding sites. Thus a preferred variant of the present invention has a modification in one or more of the positions located at a distance of 10Å to the ion-binding sites of JP170 (SEQ ID NO:1). The positions are:

20

- |    |         |                |  |
|----|---------|----------------|--|
| 25 | Site 1: | 183-189        | (i.e. positions 183, 184, 185, 186, 187, 188, 189),                |
|    |         | 191-204        | (i.e. positions 191, 192, 193, 194, 195, 196, 197, 198, 199, 200,  |
|    |         |                | 201, 202, 203, 204),   |
|    |         | 224-225;       |  |
| 30 | Site 2: | 378-393        | (i.e. positions 378, 379, 380, 381, 382, 383, 384, 385, 386, 387,  |
|    |         |                | 388, 389, 390, 391, 392, 393);                                     |
| 35 | Site 3: | 348, 350, 352, |  |
|    |         | 363-370        | (i.e. positions 363, 364, 365, 366, 367, 368, 369, 370),           |
|    |         | 380-383        | (i.e. positions 380, 381, 382, 383),                               |
|    |         | 391-400        | (i.e. positions 391, 392, 393, 394, 395, 396, 397, 398, 399, 400), |

414-420 (i.e. positions 414, 415, 416, 417, 418, 419, 420).

In detergent compositions calcium chelaters contribute to removal of calcium from the subtilases with subsequent inactivation of the enzyme as the result. To decrease the inactivation due to calcium removal of e.g. calcium chelaters variants with improved calcium stability was constructed.

Preferred variants stabilised in ion-binding site 1 are S193Q,Y; H200D,N and H200D,N+D196N.

Preferred variants stabilised in ion-binding site 2 are N390D and N391D, and preferred variants stabilised in ion-binding site 3 are G394N,Q,F,Y,S and W392S,N,Q.

### Alteration of thermostability

A variant with improved stability (typically increased thermostability) may be obtained by substitution with proline, introduction of a disulfide bond, altering a hydrogen bond contact, altering charge distribution, introduction of a salt bridge, filling in an internal structural cavity with one or more amino acids with bulkier side groups (in e.g. regions which are structurally mobile), substitution of histidine residues with other amino acids, removal of a deamidation sites, or by helix capping.

### Regions with increased mobility:

The following regions of JP170 have an increased mobility in the crystal structure of the enzyme, and it is presently believed that these regions can be responsible for stability or activity of JP170. Especially thermostabilisation may possibly be obtained by altering the highly mobile regions. Improvements of the enzyme can be obtained by mutation in the below regions and positions. Introducing e.g. larger residues or residues having more atoms in the side chain could increase the stability, or, e.g., introduction of residues having fewer atoms in the side chain could be important for the mobility and thus the activity profile of the enzyme.

Two methods are used extract the highly mobile regions from a 3D structure. One is a molecular dynamics calculation of the isotropic fluctuations, and the other is an analysis of the B-factors. The B-factors are listed in the PDB file and give a value to the uncertainty of determination of the location of the various atoms of the structure. The uncertainty relates to the mobility of the atoms in the molecules in the crystal lattice. This mobility reflects the thermal motion of the atoms and thus indicates possible sites for thermostabilisation of the enzyme.

Thus, by analysing the B-factors taken from the coordinate file in Appendix 1, (see "in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989") the following mobile regions in the JP170 structure were revealed:

5

13-18 (i.e. positions 13, 14, 15, 16, 17, 18),

37-43 (i.e. positions 37, 38, 39, 40, 41, 42, 43),

47-50 (i.e. positions 47, 48, 49, 50),

57-59 (i.e. positions 57, 58, 59),

10

96-103 (i.e. positions 96, 97, 98, 99, 100, 101, 102, 103),

131-134 (i.e. positions 131, 132, 133, 134),

152-153

162-166 (i.e. positions 162, 163, 164, 165, 166),

188-195 (i.e. positions 188, 189, 190, 191, 192, 193, 194, 195),

15

210

234-246 (i.e. positions 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246),

372-378 (i.e. positions 372, 373, 374, 375, 376, 377, 378),

387-392 (i.e. positions 387, 388, 389, 390, 391, 392),

20

406-407

419.

Molecular dynamics simulation at 300K and 400K of JP170 reveals the following highly mobile regions:

25

37-42 (i.e. positions 37, 38, 39, 40, 41, 42),

57-60 (i.e. positions 57, 58, 59, 60),

66-67,

98-103 (i.e. positions 98, 99, 100, 101, 102, 103),

107-111 (i.e. positions 107, 108, 109, 110, 111),

30

188-193 (i.e. positions 188, 189, 190, 191, 192, 193),

236-240 (i.e. positions 236, 237, 238, 239, 240),

326-332 (i.e. positions 326, 327, 328, 329, 330, 331, 332),

337-342 (i.e. positions 337, 338, 339, 340, 341, 342),

355-360 (i.e. positions 355, 356, 357, 358, 359, 360),

35

372-377 (i.e. positions 372, 373, 374, 375, 376, 377),

384-388 (i.e. positions 384, 385, 386, 387, 388),  
 404-411 (i.e. positions 404, 405, 406, 407, 408, 409, 410, 411).

Thus, a preferred JP170 subtilase variant of the present invention has been modified in one  
 5 or more of the above mentioned positions of SEQ ID NO:1. Further preferred variants com-  
 prises one or more alterations in the regions 57-60, 66-67, 107-111, 236-240, 326-332,  
 355-360, 372-377, 384-388, 404-411. Especially preferred is variant W240H,Y and variants  
 modified in the region 355-360, such as variants comprising one or more of the modifica-  
 tions: G355A,S; S356T,N; T357N,Q,D,E,P; T358S; A359S,T,N,Q and S360T,N.

10 Variants modified in the region 355-360 may be produced in accordance with the method  
 for random mutagenesis by use of the DOPE program as described herein. To obtain vari-  
 ants comprising 1-3 modifications in region 355-360 one may introduce the substitutions  
 with the following frequencies:

15	<u>wild-type</u>	<u>modified</u>
	95%	5% G355A,S
	90%	10% S356T,N
	80%	20% T357N,Q,D,E,P
	90%	10% T358S
20	80%	20% A359S,T,N,Q
	80%	20% S360T,N.

#### Disulfide bonds:

25 A JP170 variant of the present invention with improved stability, e.g. thermostability, as  
 compared to the parent JP170 subtilase may be obtained by introducing new inter-domain  
 or intra-domain bonds, such as by establishing inter- or intra-domain disulfide bridges.

Thus a further aspect of the present invention relates to a method for producing a variant of  
 a parent JP170 comprising the methods described in the paragraph "Methods of preparing  
 JP170 like or BPN' like subtilase variants" herein.

30 According to the guidelines mentioned above the below mentioned amino acid residues  
 identified in the amino acid sequence of SEQ ID NO:1 are considered as being suitable for  
 cysteine replacement. With one or more of these substitutions with cysteine, disulfide  
 bridges may possibly form in a variant of JP170. The substitutions are: G21C/A86C,  
 35 V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C,

A27C/A122C, A45C/G78C, V72C/P258C, G78C/A229C, D98C/G104C, Q111C/Y147C, G135C/G167C, R142C/P354C, V144C/A178C, G182C/P217C, A183C/G223C, A195C/Y225C, F271C/P279C, A287C/A430C, A293C/S310C, E322C/S428C, S324C/A332C, S327C/P424C, D352C/N397C, G255C/T362C, G291C/S314C.

- 5 Preferred variants comprise one or more of the substitutions: G21C/A86C, V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C, A4C/P222C and A27C/V117C.

10 Similar residues suitable for cysteine replacement in subtilases homologous with JP170 can be elucidated by finding the homologous positions in the alignment of Figure 1. Concerning another JP170 like sequence the homologous positions suitable for cysteine replacement can be selected by aligning said JP170 like sequence with all of the sequences of Figure 1 using the GAP analysis method as described above. The suitable residues can then be selected in accordance with the homologous positions in the most homologous of  
15 SEQ ID's NO:1, 2 and 3 which are the sequences of the subtilases aligned in Figure 1.

#### Surface charge distribution

A variant with improved stability (typically improved thermostability) as compared to the parent subtilase may be obtained by changing the surface charge distribution of the subtilase. For example, when the pH is lowered to about 5 or below histidine residues typically  
20 become positively charged and, consequently, unfavorable electrostatic interactions on the protein surface may occur. By engineering the surface charge of the subtilase one may avoid such unfavorable electrostatic interactions that in turn lead to a higher stability of the subtilase.

25

Therefore, a further aspect of the present invention relates to method for constructing a variant of a parent subtilase, the method comprising:

- a) identifying, on the surface of the parent subtilase, preferably a JP170 like or a BPN' like subtilase, at least one amino acid residue selected from the group consisting of Asp,  
30 Glu, Arg, Lys and His;
- b) substituting, on the surface of the parent subtilase, at least one amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His with an uncharged amino acid residue;
- c) optionally repeating steps a) and b) recursively;



- d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b);
- e) preparing the variant resulting from steps a) - d);
- f) testing the stability of said variant; and
- 5 g) optionally repeating steps a) - f) recursively; and
- h) selecting a subtilase variant having increased stability as compared to the parent subtilase.

As will be understood by the skilled person it may also, in some cases, be advantageous to substitute an uncharged amino acid residue with an amino acid residue bearing a charge or, alternatively, it may in some cases be advantageous to substitute an amino acid residue bearing a charge with an amino acid residue bearing a charge of opposite sign. Thus, the above-mentioned method may easily be employed by the skilled person also for these purposes. In the case of substituting an uncharged amino acid residue with an amino acid residue bearing a charge the above-mentioned method may be employed the only difference being steps a) and b) which will then read:

- a) identifying, on the surface of the parent subtilase, at least one uncharged amino acid residue;
- b) substituting, on the surface of the parent subtilase, at least one uncharged amino acid residue with a charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His.

Also in the case of changing the sign of an amino acid residue present on the surface of the subtilase the above method may be employed. Again, compared to the above method, the only difference being steps a) and b) which, in this case, read:

- a) identifying, on the surface of the parent subtilase, at least one charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His;
- b) substituting, on the surface of the parent subtilase, at least one charged amino acid residue identified in step a) with an amino acid residue having an opposite charge.

Thus, Asp may be substituted with Arg, Lys or His; Glu may be substituted with Arg, Lys or His; Arg may be substituted with Asp or Glu; Lys may be substituted with Asp or Glu; and His may be substituted with Asp or Glu.

In order to determine the amino acid residues of a subtilase, which are present on the surface of the enzyme, the surface accessible area are measured using the DSSP program (Kabsch and Sander, *Biopolymers* (1983), 22, 2577-2637). All residues having a surface accessibility higher than 0 is regarded a surface residue.

- 5 Amino acid residues found on the surface of JP170 using the above method are N76, N316, L381, K246, K9, K313 and K83. We consider the substitutions N79D, N316D and L381D of particular interest for stabilisation by introduction of salt bridges, whereas the substitutions K246R, K9R, K313R and K83R are of particular interest for the stabilisation at high pH.
- 10 Similar substitutions may be introduced in equivalent positions of other JP170 like subtilases.

### **Substitution with proline residues**

- 15 Improved thermostability of a subtilase can be obtained by subjecting the subtilase in question to analysis for secondary structure, identifying residues in the subtilase having dihedral angles  $\phi$  (phi) and  $\psi$  (psi) confined to the intervals  $[-90^\circ < \phi < -40^\circ$  and  $-180^\circ < \psi < 180^\circ]$ , preferably the intervals  $[-90^\circ < \phi < -40^\circ$  and  $120^\circ < \psi < 180^\circ]$  or  $[-90^\circ < \phi < -40^\circ$  and  $-50^\circ < \psi < 10^\circ]$  and excluding residues located in regions in which the subtilase is characterized by possessing  $\alpha$ -helical or  $\beta$ -sheet structure.

- 20 After the dihedral angles  $\phi$  (phi) and  $\psi$  (psi) for the amino acids have been calculated, based on the atomic structure in the crystalline subtilases, it is possible to select position(s) which has/have dihedral phi and psi angles favorable for substitution with a proline residue. The aliphatic side chain of proline residues is bonded covalently to the nitrogen atom of the peptide group. The resulting cyclic five-membered ring consequently imposes a rigid constraint on the
- 25 rotation about the N-C $_{\alpha}$  bond of the peptide backbone and simultaneously prevents the formation of hydrogen bonding to the backbone N-atom. For these structural reasons, proline residues are generally not compatible with  $\alpha$ -helical and  $\beta$ -sheet secondary conformations.

- If a proline residue is not already at the identified position(s), the naturally occurring amino acid residue is substituted with a proline residue, preferably by site directed mutagenesis applied on a gene encoding the subtilase in question.
- 30

In the group of JP170 like subtilases proline residues can advantageously be introduced at positions 22, 44, 110, 139, 140, 166, 198, 201, 203, 231, 282, 356, 357 and 378. Accordingly, a preferred JP170 variant has one or more of the substitutions: Q22P, E44P, L110P,

T139P, D140P, S166P I198P, V201P, Q203P, S231P, S282P, S356P, T357P and K378P. Especially preferred are variants comprising one or more of: E44P, Q203P and S356P.

#### Improved activity of JP170 subtilases

- 5 As mentioned the JP170 subtilases differ greatly from the BPN' like subtilases in having a long apparently non-catalytic C-terminal. A possible truncation of JP170 is the removal of approx. 115 residues including two ion-binding sites, which can be obtained by deletion of or within the region 311-433, which is non-catalytic C-terminal. Preferred deletions are of the regions 317-433 or 315-433. Preferably the new C-terminal will be within the region of  
10 311-325. Further, the deletion can be optimised with additional substitutions, such as one or more of L283N,Q; A290S,N and W306H,Y,K.

Preferred truncations comprise:

- a) deletion of region 317-433 and the substitutions L283N + A290S + W306H,  
b) deletion of region 315-433 and the substitutions L283N + A290S + W306H.

15

#### Substrate binding site

- The substrate binding site is identified by the residues in contact with a substrate model, such as the Cl2 inhibitor. The 3D structure coordinates of the JP170 subtilase with Cl2 bound in the active site can be found in Appendix 1. Without being limited to any theory, it  
20 is presently believed that binding between a substrate and an enzyme is supported by favorable interactions found within a sphere 10 Å from the substrate molecule. Examples of such favorable bonds are hydrogen bonds, strong electrostatic interaction and/or hydrophobic interactions.

- The following residues of the JP170 subtilase (SEQ ID NO:1), are within a distance of 10Å  
25 from the Cl2 inhibitor which is bound to the substrate binding site. These residues are thus believed to be involved in interactions with said substrate:

- 29-32, (i.e. residues 29, 30, 31, 32)  
64-72, (i.e. residues 64, 65, 66, 67, 68, 69, 70, 71, 72)  
93,  
30 96-98, (i.e. residues 96, 97, 98)  
100-110, (i.e. residues 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110)  
113-114,  
127-136, (i.e. residues 127, 128, 129, 130, 131, 132, 133, 134, 135, 136)  
138-141, (i.e. residues 138, 139, 140, 141)  
35 144, 157, 174,

- 180-183, (i.e. residues 180, 181, 182, 183)  
 191, 193-194,  
 202-207, (i.e. residues 202, 203, 204, 205, 206, 207)  
 211,  
 5 223-226, (i.e. residues 223, 224, 225, 226)  
 234-241, (i.e. residues 234, 235, 236, 237, 238, 239, 240, 241)  
 249-258 (i.e. residues 249, 250, 251, 252, 253, 254, 255, 256, 257, 258).

In an embodiment of the present invention a variant comprises a modification in one or  
 10 more of the above mentioned positions. A preferred variants is W129L.

#### JP170 with extra ion-binding site

The Strong ion-binding site from the BPN' subtilases can be transplanted into JP170 (or  
 other subtilases in JP170 subgroup) by deletion of N79-N82 and subsequent insertion of  
 15 LNNSIGV, followed by the substitution A45D,N and optionally the substitutions E44P,T  
 and/or R47Q.

#### Removal of ion-binding site in JP170

By removing an ion-binding site it is possible to decrease the enzymes dependency of cal-  
 20 cium in the media. The ion-binding sites in JP170 (or others from JP170 group) can be re-  
 moved with guidance from the three-dimensional structure of BPN' and Savinase (or others  
 in BPN' group), and of TY145 like subtilases.

Removal of ion-binding site 1 can be done by deletion of N186-N199 and subsequent in-  
 section of at least three amino acid residues, preferably the sequence SSN. Preferably, but  
 25 not mandatory one or both of the substitutions I7Q and V3Y is further added.

The ion-binding site 1 can be removed from a wild-type JP170 subtilase or a JP170 subti-  
 lase truncated as described above.

#### Subtilases free of ion-binding sites

30 With guidance from the three-dimensional structure of JP170 like subtilases and of TY145  
 like subtilases, the Strong and Weak ion-binding sites in BPN' like subtilases can be re-  
 moved. Likewise, as described above, with guidance from the three-dimensional structure  
 of BPN' and Savinase (or others in BPN' group), and of TY145 like subtilases, all three ion-  
 binding sites can be removed from the wild-type JP170 subtilase or from JP170 like subti-

lases. The same approach can be used to remove the ion-binding sites from TY145 like subtilases.

Exemplified in Savinase, the removal can be done by altering the loops A194-L196 and L75-L82 either by a) insertion or deletion of a number of amino acid residues in the loops or  
 5 b) by deletion of the entire loop or part of the loop and subsequent insertion of a number of residues from a corresponding loop of a JP170 or TY145 like subtilase.

Preferably the ion-binding sites of Savinase can be removed by either

- 10 i) deletion of or in the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217 and  
 deletion of or in the region L75-L82 (BPN' numbers) and insertion of at least one residue chosen from TY145 positions H83-Y92 or
- 15 ii) deletion of or in the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217 and  
 deletion of or in the region L75-L82 (BPN' numbers) and insertion of at least one residues chosen from JP170 positions N79-K83.

#### Combined modifications

20 The present invention also encompasses any of the above mentioned subtilase variants in combination with any other modification to the amino acid sequence thereof. Especially combinations with other modifications known in the art to provide improved properties to the enzyme are envisaged.

Such combinations comprise the positions: 222 (improves oxidation stability), 218 (improves thermal stability), substitutions in the  $\text{Ca}^{2+}$ -binding sites stabilizing the enzyme, e.g.  
 25 position 76, and many other apparent from the prior art.

In further embodiments a subtilase variant described herein may advantageously be combined with one or more modification(s) in any of the positions:

30 27, 36, 56, 76, 87, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 120, 123, 159, 167, 170, 206, 218, 222, 224, 232, 235, 236, 245, 248, 252 and 274 (BPN' numbering).

Specifically, the following BLSAVI, BLSUBL, BSKSMK, and BAALKP modifications are considered appropriate for combination:

35



K27R, \*36D, S56P, N76D, S87N, G97N, S101G, S103A, V104A, V104I, V104N, V104Y, H120D, N123S, G159D, Y167, R170, Q206E, N218S, M222S, M222A, T224S, A232V, K235L, Q236H, Q245R, N248D, N252K and T274A.

- 5 Furthermore variants comprising any of the modifications S101G+V104N, S87N+S101G+V104N, K27R+V104Y+N123S+T274A, N76D+S103A+V104I or N76D+V104A, or other combinations of the modifications K27R, N76D, S101G, S103A, V104N, V104Y, V104I, V104A, N123S, G159D, A232V, Q236H, Q245R, N248D, N252K, T274A in combination with any one or more of the modification(s) mentioned above exhibit  
10 improved properties.

A particular interesting variant is a variant, which, in addition to modifications according to the invention, contains the following substitutions:

S101G+S103A+V104I+G159D+A232V+Q236H+Q245R+N248D+N252K.

- 15 Moreover, subtilase variants of the main aspect(s) of the invention are preferably combined with one or more modification(s) in any of the positions 129, 131 and 194, preferably as 129K, 131H and 194P modifications, and most preferably as P129K, P131H and A194P modifications. Any of those modification(s) are expected to provide a higher expression level of the subtilase variant in the production thereof.

20

#### **Stabilization by modification of Asn-Gly pairs**

It is known that at alkaline pH, the side chain of Asn may interact with the NH group of a sequential neighbouring amino acid to form an isoAsp residue where the backbone goes through the Asp side chain. This will leave the backbone more vulnerable to proteolysis.

- 25 The deamidation is much more likely to occur if the residue that follows is a Gly. Changing the Asn in front of the Gly or the Gly will prevent this from happening and thus improve the stability, especially as concerns thermo- and storage stability.

- 30 The invention consequently further relates to a subtilase, in which either or both residues of any of the Asn-Gly sequence appearing in the amino acid sequence of the parent RP-II protease is/are deleted or substituted with a residue of a different amino acid.

The Asn and/or Gly residue may, for instance, be substituted with a residue of an amino acid selected from the group consisting of A, Q, S, P, T and Y.

35

**Modification of Tyrosine residues**

In relation to wash performance it has been found that the modification of certain tyrosine residues to phenylalanine provides an improved wash performance. Without being bound by any specific theory, it is believed that titration of these Tyr residues in the alkaline wash liquor has negative effects that are alleviated by replacing the Tyr residues with other residues, especially Phe or Trp, particularly Phe.

**Methods of preparing JP170 like or BPN' like subtilase variants**

The subtilase variants, i.e. the JP170 and BPN' variants of the present invention may be produced by any known method within the art and the present invention also relates to nucleic acid encoding a subtilase variant of the present invention, a DNA construct comprising said nucleic acid and a host cell comprising said nucleic acid sequence.

In general natural occurring proteins may be produced by culturing the organism expressing the protein and subsequently purifying the protein or it may be produced by cloning a nucleic acid, e.g. genomic DNA or cDNA, encoding the protein into an expression vector, introducing said expression vector into a host cell, culturing the host cell and purifying the expressed protein.

Typically protein variants may be produced by site-directed mutagenesis of a parent protein, introduction into expression vector, host cell etc. The parent protein may be cloned from a strain producing the polypeptide or from an expression library, i.e. it may be isolated from genomic DNA or prepared from cDNA, or a combination thereof.

In general standard procedures for cloning of genes and/or introducing mutations (random and/or site directed) into said genes may be used in order to obtain a parent subtilase, or subtilase or subtilase variant of the invention. For further description of suitable techniques reference is made to Molecular cloning: A laboratory manual (Sambrook et al. (1989), Cold Spring Harbor lab., Cold Spring Harbor, NY; Ausubel, F. M. et al. (eds.)); Current protocols in Molecular Biology (John Wiley and Sons, 1995; Harwood, C. R., and Cutting, S. M. (eds.)); Molecular Biological Methods for Bacillus (John Wiley and Sons, 1990); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M.J. Gait ed. 1984); Nucleic Acid Hybridization (B.D. Hames & S.J. Higgins eds (1985)); Transcription And Translation (B.D. Hames & S.J. Higgins, eds. (1984)); Animal Cell Culture (R.I. Freshney, ed. (1986)); Immobilized Cells And Enzymes (IRL Press, (1986)); A Practical Guide To Molecular Cloning (B. Perbal, (1984)) and WO 96/34946.

Further, variants could be constructed by:

### Random Mutagenesis

Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

The random mutagenesis of a DNA sequence encoding a parent subtilase may be conveniently performed by use of any method known in the art.

In relation to the above, a further aspect of the present invention relates to a method for generating a variant of a parent subtilase, wherein the variant exhibits an altered property, such as increased thermostability, increased stability at low pH and at low calcium concentration, relative to the parent subtilase, the method comprising:

- (a) subjecting a DNA sequence encoding the parent subtilase to random mutagenesis,
- (b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and
- (c) screening for host cells expressing a subtilase variant which has an altered property relative to the parent subtilase.

Step (a) of the above method of the invention is preferably performed using doped primers. For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents. The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues. When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleotide at the positions that are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide

can be incorporated into the DNA encoding the subtilase enzyme by any published technique, using, e.g., PCR, LCR or any DNA polymerase and ligase as deemed appropriate.

Preferably, the doping is carried out using "constant random doping", in which the percentage of wild-type and modification in each position is predefined. Furthermore, the doping

5 may be directed toward a preference for the introduction of certain nucleotides, and thereby a preference for the introduction of one or more specific amino acid residues. The doping may be made, e.g., so as to allow for the introduction of 90% wild type and 10% modifications in each position. An additional consideration in the choice of a doping scheme is based on genetic as well as protein-structural constraints. The doping scheme may be  
10 made by using the DOPE program which, *inter alia*, ensures that introduction of stop codons is avoided (L.J. Jensen et al. *Nucleic Acid Research*, 26, 697-702 (1998)).

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent subtilase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., *Technique*, 1,  
15 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., *Molec. Gen. Genet.*, 133, 1974, 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the subtilase by, e.g., transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may be subsequently transformed into the expression organism.  
20

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent subtilase. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenising agent. The  
25 DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harbored in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

30 In some cases it may be convenient to amplify the mutated DNA sequence prior to performing the expression step b) or the screening step c). Such amplification may be performed in accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

Subsequent to the incubation with or exposure to the mutagenising agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: gram positive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gram negative bacteria such as *E. coli*. The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

#### Localised random mutagenesis

The random mutagenesis may be advantageously localised to a part of the parent subtilase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

The localised or region-specific, random mutagenesis is conveniently performed by use of PCR generated mutagenesis techniques as described above or any other suitable technique known in the art. Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g., by insertion into a suitable vector, and said part may be subsequently subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

#### General method for random mutagenesis by use of the DOPE program

The random mutagenesis may be carried out by the following steps:

1. Select regions of interest for modification in the parent enzyme
2. Decide on mutation sites and non-mutated sites in the selected region
3. Decide on which kind of mutations should be carried out, e.g. with respect to the desired stability and/or performance of the variant to be constructed
4. Select structurally reasonable mutations
5. Adjust the residues selected by step 3 with regard to step 4.



6. Analyse by use of a suitable dope algorithm the nucleotide distribution.
7. If necessary, adjust the wanted residues to genetic code realism, e.g. taking into account constraints resulting from the genetic code, e.g. in order to avoid introduction of stop codons; the skilled person will be aware that some codon combinations cannot be used in practice and will need to be adapted
8. Make primers
9. Perform random mutagenesis by use of the primers
10. Select resulting subtilase variants by screening for the desired improved properties.

10 Suitable dope algorithms for use in step 6 are well known in the art. One such algorithm is described by Tomandl, D. et al., 1997, Journal of Computer-Aided Molecular Design 11:29-38. Another algorithm is DOPE (Jensen, LJ, Andersen, KV, Svendsen, A, and Kretzschmar, T (1998) Nucleic Acids Research 26:697-702).

#### 15 Expression vectors

A recombinant expression vector comprising a nucleic acid sequence encoding a subtilase variant of the invention may be any vector that may conveniently be subjected to recombinant DNA procedures and which may bring about the expression of the nucleic acid sequence.

20 The choice of vector will often depend on the host cell into which it is to be introduced. Examples of a suitable vector include a linear or closed circular plasmid or a virus. The vector may be an autonomously replicating vector, i.e., a vector which exists as an extra-chromosomal entity, the replication of which is independent of chromosomal replication, e.g., a plasmid, an extra-chromosomal element, a mini chromosome, or an artificial chromosome. The vector may contain any means for assuring self-replication. Examples of bacterial origins of replication are the origins of replication of plasmids pBR322, pUC19, pACYC177, pACYC184, pUB110, pE194, pTA1060, and pAM $\beta$ 1. Examples of origin of replications for use in a yeast host cell are the 2 micron origin of replication, the combination of CEN6 and ARS4, and the combination of CEN3 and ARS1. The origin of replication may be one having a mutation which makes it function as temperature-sensitive in the host cell (see, e.g., Ehrlich, 1978, Proceedings of the National Academy of Sciences USA 75:1433).

Alternatively, the vector may be one which, when introduced into the host cell, is integrated into the genome and replicated together with the chromosome(s) into which it has been integrated. Vectors which are integrated into the genome of the host cell may contain any

nucleic acid sequence enabling integration into the genome, in particular it may contain nucleic acid sequences facilitating integration into the genome by homologous or non-homologous recombination. The vector system may be a single vector, e.g. plasmid or virus, or two or more vectors, e.g. plasmids or virus', which together contain the total DNA to be introduced into the genome of the host cell, or a transposon.

The vector may in particular be an expression vector in which the DNA sequence encoding the subtilase variant of the invention is operably linked to additional segments or control sequences required for transcription of the DNA. The term, "operably linked" indicates that the segments are arranged so that they function in concert for their intended purposes, e.g. transcription initiates in a promoter and proceeds through the DNA sequence encoding the subtilase variant. Additional segments or control sequences include a promoter, a leader, a polyadenylation sequence, a propeptide sequence, a signal sequence and a transcription terminator. At a minimum the control sequences include a promoter and transcriptional and translational stop signals.

The promoter may be any DNA sequence that shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell.

Examples of suitable promoters for use in bacterial host cells include the promoter of the *Bacillus subtilis* levansucrase gene (sacB), the *Bacillus stearothermophilus* maltogenic amylase gene (amyM), the *Bacillus licheniformis* alpha-amylase gene (amyL), the *Bacillus amyloliquefaciens* alpha-amylase gene (amyQ), the *Bacillus subtilis* alkaline protease gene, or the *Bacillus pumilus* xylosidase gene, the *Bacillus amyloliquefaciens* BAN amylase gene, the *Bacillus licheniformis* penicillinase gene (penP), the *Bacillus subtilis* xylA and xylB genes, and the prokaryotic beta-lactamase gene (Villa-Kamaroff et al., 1978, Proceedings of the National Academy of Sciences USA 75:3727-3731). Other examples include the phage Lambda P<sub>R</sub> or P<sub>L</sub> promoters or the *E. coli* lac, trp or tac promoters or the *Streptomyces coelicolor* agarase gene (dagA). Further promoters are described in "Useful proteins from recombinant bacteria" in Scientific American, 1980, 242:74-94; and in Sambrook et al., 1989, supra.

Examples of suitable promoters for use in a filamentous fungal host cell are promoters obtained from the genes encoding *Aspergillus oryzae* TKA amylase, *Rhizomucor miehei* aspartic proteinase, *Aspergillus niger* neutral alpha-amylase, *Aspergillus niger* acid stable alpha-amylase, *Aspergillus niger* or *Aspergillus awamori* glucoamylase (glaA), *Rhizomucor miehei* lipase, *Aspergillus oryzae* alkaline protease, *Aspergillus oryzae* triose phosphate isomerase, *Aspergillus nidulans* acetamidase, *Fusarium oxysporum* trypsin-like protease

(as described in U.S. Patent No. 4,288,627, which is incorporated herein by reference), and hybrids thereof. Particularly preferred promoters for use in filamentous fungal host cells are the TAKA amylase, NA2-tpi (a hybrid of the promoters from the genes encoding *Aspergillus niger* neutral (-amylase and *Aspergillus oryzae* triose phosphate isomerase), and glaA promoters. Further suitable promoters for use in filamentous fungus host cells are the ADH3 promoter (McKnight et al., The EMBO J. 4 (1985), 2093 - 2099) or the tpiA promoter. Examples of suitable promoters for use in yeast host cells include promoters from yeast glycolytic genes (Hitzeman et al., J. Biol. Chem. 255 (1980), 12073 - 12080; Alber and Kawasaki, J. Mol. Appl. Gen. 1 (1982), 419 - 434) or alcohol dehydrogenase genes (Young et al., in Genetic Engineering of Microorganisms for Chemicals (Hollaender et al, eds.), Plenum Press, New York, 1982), or the TPI1 (US 4,599,311) or ADH2-4c (Russell et al., Nature 304 (1983), 652 - 654) promoters.

Further useful promoters are obtained from the *Saccharomyces cerevisiae* enolase (ENO-1) gene, the *Saccharomyces cerevisiae* galactokinase gene (GAL1), the *Saccharomyces cerevisiae* alcohol dehydrogenase/glyceraldehyde-3-phosphate dehydrogenase genes (ADH2/GAP), and the *Saccharomyces cerevisiae* 3-phosphoglycerate kinase gene. Other useful promoters for yeast host cells are described by Romanos et al., 1992, Yeast 8:423-488. In a mammalian host cell, useful promoters include viral promoters such as those from Simian Virus 40 (SV40), Rous sarcoma virus (RSV), adenovirus, and bovine papilloma virus (BPV).

Examples of suitable promoters for use in mammalian cells are the SV40 promoter (Subramani et al., Mol. Cell Biol. 1 (1981), 854 -864), the MT-1 (metallothionein gene) promoter (Palmiter et al., Science 222 (1983), 809 - 814) or the adenovirus 2 major late promoter.

An example of a suitable promoter for use in insect cells is the polyhedrin promoter (US 4,745,051; Vasuvedan et al., FEBS Lett. 311, (1992) 7 - 11), the P10 promoter (J.M. Vlak et al., J. Gen. Virology 69, 1988, pp. 765-776), the Autographa californica polyhedrosis virus basic protein promoter (EP 397 485), the baculovirus immediate early gene 1 promoter (US 5,155,037; US 5,162,222), or the baculovirus 39K delayed-early gene promoter (US 5,155,037; US 5,162,222).

The DNA sequence encoding a subtilase variant of the invention may also, if necessary, be operably connected to a suitable terminator.

The recombinant vector of the invention may further comprise a DNA sequence enabling the vector to replicate in the host cell in question.

The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, or a gene encoding resistance to e.g. antibiotics like ampicillin, kanamycin, chloramphenicol, erythromycin, tetracycline, spectinomycin, neomycin, hygromycin, methotrexate, or resistance to heavy metals, virus or herbicides, or which provides for prototrophy or auxotrophs. Examples of bacterial selectable markers are the *dal* genes from *Bacillus subtilis* or *Bacillus licheniformis*, resistance. A frequently used mammalian marker is the dihydrofolate reductase gene (DHFR). Suitable markers for yeast host cells are ADE2, HIS3, LEU2, LYS2, MET3, TRP1, and URA3. A selectable marker for use in a filamentous fungal host cell may be selected from the group including, but not limited to, *amdS* (acetamidase), *argB* (ornithine carbamoyltransferase), *bar* (phosphinothricin acetyltransferase), *hygB* (hygromycin phosphotransferase), *niaD* (nitrate reductase), *pyrG* (orotidine-5'-phosphate decarboxylase), *sC* (sulfate adenylyltransferase), *trpC* (anthranilate synthase), and glufosinate resistance markers, as well as equivalents from other species. Particularly, for use in an *Aspergillus* cell are the *amdS* and *pyrG* markers of *Aspergillus nidulans* or *Aspergillus oryzae* and the *bar* marker of *Streptomyces hygroscopicus*. Furthermore, selection may be accomplished by co-transformation, e.g., as described in WO 91/17243, where the selectable marker is on a separate vector.

To direct a subtilase variant of the present invention into the secretory pathway of the host cells, a secretory signal sequence (also known as a leader sequence, prepro sequence or pre sequence) may be provided in the recombinant vector. The secretory signal sequence is joined to the DNA sequence encoding the enzyme in the correct reading frame. Secretory signal sequences are commonly positioned 5' to the DNA sequence encoding the enzyme. The secretory signal sequence may be that normally associated with the enzyme or may be from a gene encoding another secreted protein.

The procedures used to ligate the DNA sequences coding for the present enzyme, the promoter and optionally the terminator and/or secretory signal sequence, respectively, or to assemble these sequences by suitable PCR amplification schemes, and to insert them into suitable vectors containing the information necessary for replication or integration, are well known to persons skilled in the art (cf., for instance, Sambrook et al.).

More than one copy of a nucleic acid sequence encoding an enzyme of the present invention may be inserted into the host cell to amplify expression of the nucleic acid sequence. Stable amplification of the nucleic acid sequence can be obtained by integrating at least one additional copy of the sequence into the host cell genome using methods well known in the art and selecting for transformants.



The nucleic acid constructs of the present invention may also comprise one or more nucleic acid sequences which encode one or more factors that are advantageous in the expression of the polypeptide, e.g., an activator (e.g., a trans-acting factor), a chaperone, and a processing protease. Any factor that is functional in the host cell of choice may be used in the present invention. The nucleic acids encoding one or more of these factors are not necessarily in tandem with the nucleic acid sequence encoding the polypeptide.

#### Host cells

The DNA sequence encoding a subtilase variant of the present invention may be either homologous or heterologous to the host cell into which it is introduced. If homologous to the host cell, i.e. produced by the host cell in nature, it will typically be operably connected to another promoter sequence or, if applicable, another secretory signal sequence and/or terminator sequence than in its natural environment. The term "homologous" is intended to include a DNA sequence encoding an enzyme native to the host organism in question. The term "heterologous" is intended to include a DNA sequence not expressed by the host cell in nature. Thus, the DNA sequence may be from another organism, or it may be a synthetic sequence.

The host cell into which the DNA construct or the recombinant vector of the invention is introduced may be any cell that is capable of producing the present subtilase variants, such as prokaryotes, e.g. bacteria or eukaryotes, such as fungal cells, e.g. yeasts or filamentous fungi, insect cells, plant cells or mammalian cells.

Examples of bacterial host cells which, on cultivation, are capable of producing the subtilase variants of the invention are gram-positive bacteria such as strains of *Bacillus*, e.g. strains of *B. subtilis*, *B. licheniformis*, *B. lentus*, *B. brevis*, *B. stearothermophilus*, *B. alkalophilus*, *B. amyloliquefaciens*, *B. coagulans*, *B. circulans*, *B. lautus*, *B. megaterium* or *B. thuringiensis*, or strains of *Streptomyces*, such as *S. lividans* or *S. murinus*, or gram-negative bacteria such as *Escherichia coli* or *Pseudomonas sp.*

The transformation of the bacteria may be effected by protoplast transformation, electroporation, conjugation, or by using competent cells in a manner known per se (cf. Sambrook et al., supra).

When expressing the subtilase variant in bacteria such as *E. coli*, the enzyme may be retained in the cytoplasm, typically as insoluble granules (known as inclusion bodies), or it may be directed to the periplasmic space by a bacterial secretion sequence. In the former case, the cells are lysed and the granules are recovered and denatured after which the enzyme is refolded by diluting the denaturing agent. In the latter case, the enzyme may be



recovered from the periplasmic space by disrupting the cells, e.g. by sonication or osmotic shock, to release the contents of the periplasmic space and recovering the enzyme.

When expressing the subtilase variant in gram-positive bacteria such as *Bacillus* or *Streptomyces* strains, the enzyme may be retained in the cytoplasm, or it may be directed to the extracellular medium by a bacterial secretion sequence. In the latter case, the enzyme may be recovered from the medium as described below.

Examples of host yeast cells include cells of a species of *Candida*, *Kluyveromyces*, *Saccharomyces*, *Schizosaccharomyces*, *Pichia*, *Hansenula*, or *Yarrowia*. In a particular embodiment, the yeast host cell is a *Saccharomyces carlsbergensis*, *Saccharomyces cerevisiae*, *Saccharomyces diastaticus*, *Saccharomyces douglasii*, *Saccharomyces kluyveri*, *Saccharomyces norbensis* or *Saccharomyces oviformis* cell. Other useful yeast host cells are a *Kluyveromyces lactis*, *Kluyveromyces fragilis*, *Hansenula polymorpha*, *Pichia pastoris*, *Yarrowia lipolytica*, *Schizosaccharomyces pombe*, *Ustilago maylis*, *Candida maltose*, *Pichia guilliermondii* and *Pichia methanolio* cell (cf. Gleeson et al., J. Gen. Microbiol. 132, 1986, pp. 3459-3465; US 4,882,279 and US 4,879,231). Since the classification of yeast may change in the future, for the purposes of this invention, yeast shall be defined as described in Biology and Activities of Yeast (Skinner, F.A., Passmore, S.M., and Davenport, R.R., eds, Soc. App. Bacteriol. Symposium Series No. 9, 1980. The biology of yeast and manipulation of yeast genetics are well known in the art (see, e.g., Biochemistry and Genetics of Yeast, Bacil, M., Horecker, B.J., and Stopani, A.O.M., editors, 2nd edition, 1987; The Yeasts, Rose, A.H., and Harrison, J.S., editors, 2nd edition, 1987; and The Molecular Biology of the Yeast *Saccharomyces*, Strathern et al., editors, 1981). Yeast may be transformed using the procedures described by Becker and Guarente, In Abelson, J.N. and Simon, M.I., editors, Guide to Yeast Genetics and Molecular Biology, Methods in Enzymology, Volume 194, pp 182-187, Academic Press, Inc., New York; Ito et al., 1983, Journal of Bacteriology 153:163; and Hinnen et al., 1978, Proceedings of the National Academy of Sciences USA 75:1920.

Examples of filamentous fungal cells include filamentous forms of the subdivision Eumycota and Oomycota (as defined by Hawksworth et al., 1995, supra), in particular it may of the a cell of a species of *Acremonium*, such as *A. chrysogenum*, *Aspergillus*, such as *A. awamori*, *A. foetidus*, *A. japonicus*, *A. niger*, *A. nidulans* or *A. oryzae*, *Fusarium*, such as *F. bactridioides*, *F. cerealis*, *F. crookwellense*, *F. culmorum*, *F. graminearum*, *F. graminum*, *F. heterosporum*, *F. negundi*, *F. reticulatum*, *F. roseum*, *F. sambucinum*, *F. sarcochroum*, *F. sulphureum*, *F. trichothecioides* or *F. oxysporum*, *Humicola*, such as *H. insolens* or *H. lanuginosa*, *Mucor*, such as *M. miehei*, *Myceliophthora*, such as *M. thermophilum*, *Neuro-*

spora, such as *N. crassa*, *Penicillium*, such as *P. purpurogenum*, *Thielavia*, such as *T. terrestris*, *Tolypocladium*, or *Trichoderma*, such as *T. harzianum*, *T. koningii*, *T. longibrachiatum*, *T. reesei* or *T. viride*, or a teleomorph or synonym thereof. The use of *Aspergillus spp.* for the expression of proteins is described in, e.g., EP 272 277, EP 230 023.

- 5 Examples of insect cells include a *Lepidoptera* cell line, such as *Spodoptera frugiperda* cells or *Trichoplusia ni* cells (cf. US 5,077,214). Culture conditions may suitably be as described in WO 89/01029 or WO 89/01028. Transformation of insect cells and production of heterologous polypeptides therein may be performed as described in US 4,745,051; US 4,775,624; US 4,879,236; US 5,155,037; US 5,162,222; EP 397,485).
- 10 Examples of mammalian cells include Chinese hamster ovary (CHO) cells, HeLa cells, baby hamster kidney (BHK) cells, COS cells, or any number of other immortalized cell lines available, e.g., from the American Type Culture Collection. Methods of transfecting mammalian cells and expressing DNA sequences introduced in the cells are described in e.g. Kaufman and Sharp, J. Mol. Biol. 159 (1982), 601 - 621; Southern and Berg, J. Mol. Appl. Genet. 1 (1982), 327 - 341; Loyter et al., Proc. Natl. Acad. Sci. USA 79 (1982), 422 - 426; Wigler et al., Cell 14 (1978), 725; Corsaro and Pearson, Somatic Cell Genetics 7 (1981), 603; Ausubel et al., Current Protocols in Molecular Biology, John Wiley and Sons, Inc., N.Y., 1987, Hawley-Nelson et al., Focus 15 (1993), 73; Ciccarone et al., Focus 15 (1993), 80; Graham and van der Eb, Virology 52 (1973), 456; and Neumann et al., EMBO J. 1 (1982), 841 - 845. Mammalian cells may be transfected by direct uptake using the calcium phosphate precipitation method of Graham and Van der Eb (1978, Virology 52:546).
- 20

#### Methods for expression and isolation of proteins

- 25 To express an enzyme of the present invention the above mentioned host cells transformed or transfected with a vector comprising a nucleic acid sequence encoding an enzyme of the present invention are typically cultured in a suitable nutrient medium under conditions permitting the production of the desired molecules, after which these are recovered from the cells, or the culture broth.

- The medium used to culture the host cells may be any conventional medium suitable for growing the host cells, such as minimal or complex media containing appropriate supplements. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. in catalogues of the American Type Culture Collection). The media may be prepared using procedures known in the art (see, e.g., references for bacteria and yeast; Bennett, J.W. and LaSure, L., editors, More Gene Manipulations in Fungi, Academic Press, CA, 1991).
- 30
- 35

If the enzymes of the present invention are secreted into the nutrient medium, they may be recovered directly from the medium. If they are not secreted, they may be recovered from cell lysates. The enzymes of the present invention may be recovered from the culture medium by conventional procedures including separating the host cells from the medium by centrifugation or filtration, precipitating the proteinaceous components of the supernatant or filtrate by means of a salt, e.g. ammonium sulphate, purification by a variety of chromatographic procedures, e.g. ion exchange chromatography, gelfiltration chromatography, affinity chromatography, or the like, dependent on the enzyme in question.

The enzymes of the invention may be detected using methods known in the art that are specific for these proteins. These detection methods include use of specific antibodies, formation of a product, or disappearance of a substrate. For example, an enzyme assay may be used to determine the activity of the molecule. Procedures for determining various kinds of activity are known in the art.

The enzymes of the present invention may be purified by a variety of procedures known in the art including, but not limited to, chromatography (e.g., ion exchange, affinity, hydrophobic, chromatofocusing, and size exclusion), electrophoretic procedures (e.g., preparative isoelectric focusing (IEF), differential solubility (e.g., ammonium sulfate precipitation), or extraction (see, e.g., Protein Purification, J-C Janson and Lars Ryden, editors, VCH Publishers, New York, 1989).

When an expression vector comprising a DNA sequence encoding an enzyme of the present invention is transformed/transfected into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme. An advantage of using a heterologous host cell is that it is possible to make a highly purified enzyme composition, characterized in being free from homologous impurities, which are often present when a protein or peptide is expressed in a homologous host cell. In this context homologous impurities mean any impurity (e.g. other polypeptides than the enzyme of the invention) which originates from the homologous cell where the enzyme of the invention is originally obtained from.

### DETERGENT APPLICATIONS

The enzyme of the invention may be added to and thus become a component of a detergent composition.

The detergent composition of the invention may for example be formulated as a hand or machine laundry detergent composition including a laundry additive composition suitable for pre-treatment of stained fabrics and a rinse added fabric softener composition, or be

formulated as a detergent composition for use in general household hard surface cleaning operations, or be formulated for hand or machine dishwashing operations.

In a specific aspect, the invention provides a detergent additive comprising the enzyme of the invention. The detergent additive as well as the detergent composition may comprise  
 5 one or more other enzymes such as a protease, a lipase, a cutinase, an amylase, a carbohydrate, a cellulase, a pectinase, a mannanase, an arabinase, a galactanase, a xylanase, an oxidase, e.g., a laccase, and/or a peroxidase.

In general the properties of the chosen enzyme(s) should be compatible with the selected detergent, (i.e. pH-optimum, compatibility with other enzymatic and non-enzymatic ingredi-  
 10 ents, etc.), and the enzyme(s) should be present in effective amounts.

Proteases: Suitable proteases include those of animal, vegetable or microbial origin. Microbial origin is preferred. Chemically modified or protein engineered mutants are included. The protease may be a serine protease or a metallo protease, preferably an alkaline microbial protease or a trypsin-like protease. Examples of alkaline proteases are subtilisins,  
 15 especially those derived from *Bacillus*, e.g., subtilisin Novo, subtilisin Carlsberg, subtilisin 309, subtilisin 147 and subtilisin 168 (described in WO 89/06279). Examples of trypsin-like proteases are trypsin (e.g. of porcine or bovine origin) and the *Fusarium* protease described in WO 89/06270 and WO 94/25583.

Examples of useful proteases are the variants described in WO 92/19729, WO 98/20115, WO 98/20116, and WO 98/34946, especially the variants with substitutions in one or more of the following positions: 27, 36, 57, 76, 87, 97, 101, 104, 120, 123, 167, 170, 194, 206,  
 20 218, 222, 224, 235 and 274.

Preferred commercially available protease enzymes include Alcalase™, Savinase™, Primase™, Duralase™, Esperase™, and Kannase™ (Novo Nordisk A/S), Maxatase™, Maxacal™, Maxapem™, Properase™, Purafect™, Purafect OxP™, FN2™, and FN3™ (Genencor International Inc.).  
 25

Lipases: Suitable lipases include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful lipases include lipases from  
 30 *Humicola* (synonym *Thermomyces*), e.g. from *H. lanuginosa* (*T. lanuginosus*) as described in EP 258 068 and EP 305 216 or from *H. insolens* as described in WO 96/13580, a *Pseudomonas* lipase, e.g. from *P. alcaligenes* or *P. pseudoalcaligenes* (EP 218 272), *P. cepacia* (EP 331 376), *P. stutzeri* (GB 1,372,034), *P. fluorescens*, *Pseudomonas* sp. strain  
 35 SD 705 (WO 95/06720 and WO 96/27002), *P. wisconsinensis* (WO 96/12012), a *Bacillus*



lipase, e.g. from *B. subtilis* (Dartois et al. (1993), *Biochemica et Biophysica Acta*, 1131, 253-360), *B. stearothermophilus* (JP 64/744992) or *B. pumilus* (WO 91/16422).

Other examples are lipase variants such as those described in WO 92/05249, WO 94/01541, EP 407 225, EP 260 105, WO 95/35381, WO 96/00292, WO 95/30744, WO 94/25578, WO 95/14783, WO 95/22615, WO 97/04079 and WO 97/07202.

Preferred commercially available lipase enzymes include Lipolase™ and Lipolase Ultra™ (Novo Nordisk A/S).

Amylases: Suitable amylases ( $\alpha$  and/or  $\beta$ ) include those of bacterial or fungal origin.

Chemically modified or protein engineered mutants are included. Amylases include, for example,  $\alpha$ -amylases obtained from *Bacillus*, e.g. a special strain of *B. licheniformis*, described in more detail in GB 1,296,839.

Examples of useful amylases are the variants described in WO 94/02597, WO 94/18314, WO 96/23873, and WO 97/43424, especially the variants with substitutions in one or more of the following positions: 15, 23, 105, 106, 124, 128, 133, 154, 156, 181, 188, 190, 197, 202, 208, 209, 243, 264, 304, 305, 391, 408, and 444.

Commercially available amylases are Duramyl™, Termamyl™, Fungamyl™ and BAN™ (Novo Nordisk A/S), Rapidase™ and Purastar™ (from Genencor International Inc.).

Cellulases: Suitable cellulases include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Suitable cellulases include cellulases from the genera *Bacillus*, *Pseudomonas*, *Humicola*, *Fusarium*, *Thielavia*, *Acremonium*, e.g. the fungal cellulases produced from *Humicola insolens*, *Myceliophthora thermophila* and *Fusarium oxysporum* disclosed in US 4,435,307, US 5,648,263, US 5,691,178, US 5,776,757 and WO 89/09259.

Especially suitable cellulases are the alkaline or neutral cellulases having colour care benefits. Examples of such cellulases are cellulases described in EP 0 495 257, EP 0 531 372, WO 96/11262, WO 96/29397, WO 98/08940. Other examples are cellulase variants such as those described in WO 94/07998, EP 0 531 315, US 5,457,046, US 5,686,593, US 5,763,254, WO 95/24471, WO 98/12307 and PCT/DK98/00299.

Commercially available cellulases include Celluzyme™, and Carezyme™ (Novo Nordisk A/S), Clazinase™, and Puradax HA™ (Genencor International Inc.), and KAC-500(B)™ (Kao Corporation).



Peroxidases/Oxidases: Suitable peroxidases/oxidases include those of plant, bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful peroxidases include peroxidases from *Coprinus*, e.g. from *C. cinereus*, and variants thereof as those described in WO 93/24618, WO 95/10602, and WO 98/15257.

- 5 Commercially available peroxidases include Guardzyme™ (Novo Nordisk A/S).

The detergent enzyme(s) may be included in a detergent composition by adding separate additives containing one or more enzymes, or by adding a combined additive comprising all of these enzymes. A detergent additive of the invention, i.e. a separate additive or a com-  
10 bined additive, can be formulated e.g. as a granulate, a liquid, a slurry, etc. Preferred detergent additive formulations are granulates, in particular non-dusting granulates, liquids, in particular stabilized liquids, or slurries.

Non-dusting granulates may be produced, e.g., as disclosed in US 4,106,991 and 4,661,452 and may optionally be coated by methods known in the art. Examples of waxy  
15 coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to 20000; ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and mono- and di- and triglycerides of fatty acids. Examples of film-forming coating materials  
20 suitable for application by fluid bed techniques are given in GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods. Protected enzymes may be prepared according to the method disclosed in EP 238,216.

- 25 The detergent composition of the invention may be in any convenient form, e.g., a bar, a tablet, a powder, a granule, a paste or a liquid. A liquid detergent may be aqueous, typically containing up to 70 % water and 0-30 % organic solvent, or non-aqueous.

The detergent composition comprises one or more surfactants, which may be non-ionic in-  
30 cluding semi-polar and/or anionic and/or cationic and/or zwitterionic. The surfactants are typically present at a level of from 0.1% to 60% by weight.

When included therein the detergent will usually contain from about 1% to about 40% of an anionic surfactant such as linear alkylbenzenesulfonate, alpha-olefinsulfonate, alkyl sulfate (fatty alcohol sulfate), alcohol ethoxysulfate, secondary alkanesulfonate, alpha-sulfo fatty  
35 acid methyl ester, alkyl- or alkenylsuccinic acid or soap.

When included therein the detergent will usually contain from about 0.2% to about 40% of a non-ionic surfactant such as alcohol ethoxylate, nonylphenol ethoxylate, alkylpolyglycoside, alkyldimethylamineoxide, ethoxylated fatty acid monoethanolamide, fatty acid monoethanolamide, polyhydroxy alkyl fatty acid amide, or N-acyl N-alkyl derivatives of glucosamine ("glucamides").

The detergent may contain 0-65 % of a detergent builder or complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, carbonate, citrate, nitrilotriacetic acid, ethylenediaminetetraacetic acid, diethylenetriaminepentaacetic acid, alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst).

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose, poly(vinylpyrrolidone), poly (ethylene glycol), poly(vinyl alcohol), poly(vinylpyridine-N-oxide), poly(vinylimidazole), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise a  $H_2O_2$  source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetythylenediamine or nonanoyloxybenzenesulfonate. Alternatively, the bleaching system may comprise peroxyacids of e.g. the amide, imide, or sulfone type.

The enzyme(s) of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g., a polyol such as propylene glycol or glycerol, a sugar or sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g., an aromatic borate ester, or a phenyl boronic acid derivative such as 4-formylphenyl boronic acid, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, hydrotropes, tarnish inhibitors, or perfumes.

In the detergent compositions any enzyme, in particular the enzyme of the invention, may be added in an amount corresponding to 0.01-100 mg of enzyme protein per litre of wash

liquor, preferably 0.05-5 mg of enzyme protein per litre of wash liquor, in particular 0.1-1 mg of enzyme protein per litre of wash liquor.

The enzyme of the invention may additionally be incorporated in the detergent formulations disclosed in WO 97/07202 which is hereby incorporated as reference.

5

## **MATERIALS AND METHODS**

### **Textiles**

Standard textile pieces are obtained from EMPA St. Gallen, Lerchfeldstrasse 5, CH-9014 St. Gallen, Switzerland. Especially type EMPA 116 (cotton textile stained with blood, milk and ink) and EMPA 117 (polyester/cotton textile stained with blood, milk and ink).

### **Method for producing a subtilase variant**

The present invention provides a method of producing an isolated enzyme according to the invention, wherein a suitable host cell, which has been transformed with a DNA sequence encoding the enzyme, is cultured under conditions permitting the production of the enzyme, and the resulting enzyme is recovered from the culture.

When an expression vector comprising a DNA sequence encoding the enzyme is transformed into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme of the invention. Thereby it is possible to make a highly purified subtilase composition, characterized in being free from homologous impurities.

The medium used to culture the transformed host cells may be any conventional medium suitable for growing the host cells in question. The expressed subtilase may conveniently be secreted into the culture medium and may be recovered there-from by well-known procedures including separating the cells from the medium by centrifugation or filtration, precipitating proteinaceous components of the medium by means of a salt such as ammonium sulfate, followed by chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

30

## **EXAMPLE 1**

### Removal of ion-binding sites from BPN' like subtilases

The below mentioned regions in JP170 and TY145 have been selected for transfer from JP170 and TY145 to Savinase. By use of the molecular methods of preparing subtilase variants as described herein, the Savinase regions (BPN' numbering) are deleted and the

35

JP170 and TY145 regions are inserted instead. Since the Savinase regions are in contact with ion-binding sites, the purpose of the modifications is to remove the ion-binding site from Savinase.

5 Savinase region A194-L196  
 JP170 region P209-P217 and  
 Savinase region L75-L82  
 TY145 region H83-Y92,

10 alternatively the modification can be

Savinase region A194-L196  
 JP170 region P209-P217 and  
 Savinase region L75-L82  
 15 JP170 region N79-K83.

## EXAMPLE 2

### Purification and assessment of enzyme concentration

After fermentation, purification of subtilisin variants is accomplished using Hydrophobic  
 20 Charge Induction Chromatography (HCIC) and subsequent vacuum filtration.  
 To capture the enzyme, the HCIC uses a cellulose matrix to which 4-Mercapto-Ethyl-  
 Pyridine (4-MEP) is bound.

Beads of the cellulose matrix sized 80-100  $\mu\text{m}$  are mixed with a media containing yeast  
 25 and the transformed *B. subtilis* capable of secreting the subtilisin variants and incubated at  
 pH 9.5 in Unifilter<sup>®</sup> microplates.

As 4-MEP is hydrophobic at pH > 7 and the subtilisin variants are hydrophobic at pH 9.5 a  
 hydrophobic association is made between the secreted enzyme and the 4-MEP on the  
 beads. After incubation the media and cell debris is removed by vacuum filtration while the  
 30 beads and enzyme are kept on the filter.

To elute the enzyme from the beads the pH is now lowered by washing the filter with an  
 elution buffer (pH 5). Hereby the enzymes part from the beads and can be retrieved from  
 the buffer.

The concentration of the purified subtilisin enzyme variants is assessed by active site titration (AST).

The purified enzyme is incubated with the high affinity inhibitor Cl-2A at different concentrations to inhibit a varying amount of the active sites. The protease and inhibitor binds to each other at a 1:1 ratio and accordingly the enzyme concentration can be directly related to the concentration of inhibitor, at which all protease is inactive. To measure the residual protease activity, a substrate (0.6 mM Suc-Ala-Ala-Pro-Phe-pNA in Tris/HCl buffer) is added after the incubation with inhibitor and during the following 4 minutes the development of the degradation product pNA (paranitrophenol) is measured periodically at 405 nm on an Elisa Reader.

### EXAMPLE 3

#### Wash performance of detergent compositions comprising modified enzymes

Wash performance of detergent compositions comprising enzyme hybrids or enzyme variants of the present is tested at low washing temperature.

### AMSA

The enzyme variants of the present application are tested using the Automatic Mechanical Stress Assay (AMSA). With the AMSA test the wash performance of a large quantity of small volume enzyme-detergent solutions can be examined. The AMSA plate has a number of slots for test solutions and a lid firmly squeezing the textile swatch to be washed against all the slot openings. During the washing time, the plate, test solutions, textile and lid are vigorously shaken to bring the test solution in contact with the textile and apply mechanical stress. For further description see WO 02/42740 especially the paragraph "Special method embodiments" at page 23-24.

The assay is conducted under the experimental conditions specified below:

Detergent base	Standard European detergent
Detergent dosage	1.5 g/l
Test solution volume	160 micro l
pH	10-10.5 adjusted with NaHCO <sub>3</sub>
Wash time	12 minutes
Temperature	20°C



Water hardness	9°dH
Enzyme concentration in test solution	5 nM, 10 nM and 30 nM
Test material	EMPA 117

After washing the textile pieces are flushed in tap water and air-dried.

The performance of the enzyme variant is measured as the brightness of the colour of the textile samples washed with that specific enzyme variant. Brightness can also be expressed as the intensity of the light reflected from the textile sample when luminated with white light. When the textile is stained the intensity of the reflected light is lower, than that of a clean textile. Therefore the intensity of the reflected light can be used to measure wash performance of an enzyme variant.

Colour measurements are made with a professional flatbed scanner (*PFU DL2400pro*), which is used to capture an image of the washed textile samples. The scans are made with a resolution of 200 dpi and with an output colour dept of 24 bits. In order to get accurate results, the scanner is frequently calibrated with a *Kodak reflective IT8 target*.

To extract a value for the light intensity from the scanned images, a special designed software application is used (*Novozymes Color Vector Analyzer*). The program retrieves the 24 bit pixel values from the image and converts them into values for red, green and blue (RGB). The intensity value (Int) is calculated by adding the RGB values together as vectors and then taking the length of the resulting vector:

$$Int = \sqrt{r^2 + g^2 + b^2}$$

The wash performance (P) of the variants is calculated in accordance with the below formula:

$$P = Int(v) - Int(r)$$

where

Int(v) is the light intensity value of textile surface washed with enzyme variant and Int(r) is the light intensity value of textile surface washed with the reference enzyme e.g. subtilisin 309 (BLSAVI).

Performance Scores (S) are summing up the performances (P) of the tested enzyme variants as:

S (2) which indicates that the variant performs better than the reference at all three

concentrations (5, 10 and 30 nM) and

S (1) which indicates that the variant performs better than the reference at one or two concentrations.

## 5 Mini wash assay

A millilitre scale wash performance assay is conducted under the following conditions:

Detergent base	Standard European detergent powder
Detergent dose	1.5 g/l
pH	"as is" in the current detergent solution and is not adjusted.
Wash time	14 min.
Temperature	20°C
Water hardness	9°dH, adjusted by adding $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$ ; $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ ; $\text{NaHCO}_3$ ( $\text{Ca}^{2+}:\text{Mg}^{2+}:\text{HCO}_3^- = 2:1:6$ ) to milli-Q water.
Enzyme conc.	5 nM, 10 nM
Test system	125 ml glass beakers. Textile dipped in test solution. Continuously up and down, 50 times per minute
Textile/volume	1 textile piece (13 x 3 cm) in 50 ml test solution
Test material	EMPA 117 textile swatches

After wash the measurement of remission from the test material is done at 460 nm using a Zeiss MCS 521 VIS spectrophotometer. The measurements are done according to the manufacturer's protocol.

## CLAIMS

1. A JP170 like subtilase which is at least 58% homologous to the sequence of SEQ ID NO:1, comprising the overall subtilisin fold and the following structural characteristics:

- 5 a) a twisted beta-sheet with 7 strands,  
b) six alpha helices,  
c) three ion-binding sites,  
and not comprising the Strong and Weak ion-binding sites of the BPN' like subtilases, and with the exception of the subtilases JP170, KP1790, KP9860, KP43, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233.

2. The subtilase of claim 1, wherein the positions of said three ion-binding sites in the three-dimensional structure of the subtilase is defined by the distance to the c-alpha atoms of the three active site amino acid residues of the subtilases, that is Ser, His and Asp, and the c-alpha atom of the amino acid residue next to the active site Ser residue (next to Ser), wherein said distances between:

- 15 a) ion-binding site 1 and i) Asp c-alpha atom is 26.70-28.70Å, ii) His c-alpha atom is 22.10-24.10Å, iii) Ser c-alpha atom is 16.95-18.95Å, iv) next to Ser c-alpha atom is 15.30-17.30Å,  
20 b) ion-binding site 2 and i) Asp c-alpha atom is 33.50-35.50Å, ii) His c-alpha atom is 37-39Å, iii) Ser c-alpha atom is 29.40-31.40Å, iv) next to Ser c-alpha atom is 30.70-32.70Å,  
25 c) ion-binding site 3 and i) Asp c-alpha atom is 41.50-43.50Å, ii) His c-alpha atom is 42.90-44.90Å, iii) Ser c-alpha atom is 34.50-36.50Å, iv) next to Ser c-alpha atom is 35-37Å.

3. A subtilase according to claim 2 wherein the positions of the three ion-binding sites are defined by the distance to the c-alpha atoms of amino acid residues Asp30, His68, Ser254 and Met255 of SEQ ID NO:1 or by the distances to the c-alpha atoms of equivalent amino acid residues in another subtilase of the invention in accordance with claim 1, wherein the distance between

- 30 a) ion-binding site 1 and i) Asp c-alpha atom is 27.69Å, ii) His c-alpha atom is 23.12Å, iii) Ser c-alpha atom is 17.95Å, iv) next to Ser c-alpha atom is 16.34Å,  
35 b) ion-binding site 2 and i) Asp c-alpha atom is 34.49Å, ii) His c-alpha atom is 38.03Å, iii)

Ser c-alpha atom is 30.41Å, iv) next to Ser c-alpha atom is 31.68Å,  
 c) ion-binding site 3 and i) Asp c-alpha atom is 42.48Å, ii) His c-alpha atom is 43.87Å, iii)  
 Ser c-alpha atom is 35.51Å, iv) next to Ser c-alpha atom is 36.02Å,  
 and wherein the variation on the above mentioned distances are  $\pm 0.80\text{\AA}$ , preferably  
 5  $\pm 0.70\text{\AA}$ , more preferably  $\pm 0.60\text{\AA}$ , more preferably  $\pm 0.50\text{\AA}$ , more preferably  $\pm 0.40\text{\AA}$ , or most  
 preferably  $\pm 0.30\text{\AA}$ .

4. A method of producing a variant of a parent JP170 like subtilase, the variant having at  
 least one altered property as compared to the parent JP170 like subtilase, the method  
 10 comprising:

- a) modelling the parent JP170 like subtilase on the three-dimensional structure of a  
 JP170 subtilase to produce a three-dimensional structure of the parent JP170 like sub-  
 tilase;
- b) identifying on the basis of the comparison in step a) at least one structural part of the  
 15 parent JP170 subtilase, wherein an alteration in said structural part is predicted to re-  
 sult in an altered property;
- c) modifying the nucleic acid sequence encoding the parent JP170 subtilase to produce a  
 nucleic acid sequence encoding deletion or substitution of one or more amino acids at  
 a position corresponding to said structural part, or an insertion of one or more amino  
 20 acid residues in positions corresponding to said structural part;
- d) expressing the modified nucleic acid sequence in a host cell to produce the variant  
 JP170 subtilase;
- e) isolating the produced subtilase;
- f) purifying the isolated subtilase and
- 25 g) recovering the purified subtilase.

5. A method according to claim 4, wherein the JP170 subtilase on which the parent JP170  
 subtilase is modelled in step a) is at least 58% homologous to SEQ ID NO:1, preferably at  
 least 60% homologous, more preferably at least 65%, more preferably at least 70%, more  
 30 preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more  
 preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more  
 preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more  
 preferably at least 96%, more preferably at least 97%, more preferably at least 98% or  
 even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

6. A method according to claim 4 or 5, wherein the JP170 subtilase on which the parent JP170 subtilase is modelled in step a) is defined in accordance with claim 3.

7. A method of producing a variant of a parent Subtilisin family subtilase, the variant having at least one altered property as compared to the parent Subtilisin family subtilase, the method comprising:

a) modelling the parent Subtilisin family subtilase on the three-dimensional structure of a Subtilisin family subtilase to produce a three-dimensional structure of the parent Subtilisin family subtilase;

b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a JP170 like subtilase;

c) identifying on the basis of the comparison in step b) at least one structural part of the parent Subtilisin family subtilase, wherein an alteration in said structural part is predicted to result in an altered property;

d) modifying the nucleic acid sequence encoding the parent Subtilisin family subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;

e) expressing the modified nucleic acid sequence in a host cell to produce the variant Subtilisin family subtilase,

f) isolating the produced subtilase,

g) purifying the isolated subtilase and

h) recovering the purified subtilase.

8. A method according to claim 7, wherein the Subtilisin family subtilase on which the parent Subtilisin family subtilase is modelled in step a) is at least 61% homologous to SEQ ID NO:4, preferably at least 63% homologous, preferably at least 65% homologous, more preferably at least 70%, more preferably at least 74%, more preferably at least 80%, more preferably at least 83%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:4.



9. A method according to any of claim 7 and 8, wherein the JP170 subtilase of step b) is defined in accordance with claim 3.

10. A method according to any of claims 7-9, wherein the JP170 subtilase in step b) is at least 58% homologous with the sequence of SEQ ID NO:1, preferably at least 60% homologous, more preferably at least 65%, more preferably at least 70%, more preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

11. A method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

- a) modelling the parent JP170 like subtilase on the three-dimensional structure of a JP170 like subtilase to produce a three-dimensional structure of the parent JP170 like subtilase;
- b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a Subtilisin family subtilase;
- c) identifying on the basis of the comparison in step b) at least one structural part of the parent JP170 like subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
- d) modifying the nucleic acid sequence encoding the parent JP170 like subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
- e) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 like subtilase;
- f) isolating the produced subtilase;
- g) purifying the isolated subtilase and
- h) recovering the purified subtilase.

12. A method according to claim 11, wherein the Subtilisin family subtilase of step b) is at least 61% homologous to SEQ ID NO:4, preferably at least 63% homologous, preferably at

least 65% homologous, more preferably at least 70%, more preferably at least 74%, more preferably at least 80%, more preferably at least 83%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:4.

13. A method according to any of claim 11 and 12, wherein the parent JP170 like subtilase is defined in accordance with claim 3.

14. A method according to any of claims 11-13, wherein the parent JP170 like subtilase is at least 58% homologous with the sequence of SEQ ID NO:1, preferably at least 60% homologous, more preferably at least 65%, more preferably at least 70%, more preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

15. A variant subtilase comprising an alteration in one or more positions located at a distance of not more than 10Å to one of the ion-binding sites of JP170, wherein the positions, as specified in SEQ ID NO:1, located at a distance of not more than 10Å to:

- a) ion-binding site 1 are: 183, 184, 185, 186, 187, 188, 189, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 224 and 225,
- b) ion-binding site 2 are: 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392 and 393,
- c) ion-binding site 3 are: 348, 350, 352, 363, 364, 365, 366, 367, 368, 369, 370, 380, 381, 382, 383, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 414, 415, 416, 417, 418, 419, 420.

16. A subtilase variant according to claim 15 comprising one or more of the substitutions: S193Q,Y; H200D,N; H200D,N+D196N; N390D; N391D; G394N,Q,F,Y,S and W392S,N,Q.

17. A JP170 like subtilase variant comprising the introduction of a ion-binding site corresponding to the Strong ion-binding site of the BPN' like family subtilases, wherein said vari-

ant has a deletion of or in the region N79-N82 of SEQ ID NO:1 and subsequent insertion of one or more amino acid residues, preferably insertion of the sequence LNNSIQV followed by the substitution A45D,N and optionally the substitutions E44P,T and/or R47Q.

- 5 18. A JP170 like subtilase variant in which one or more ion-binding sites have been removed, wherein said variant comprises deletion of or in the region N186-N199 of SEQ ID NO:1 and subsequent insertion of one or more amino acid residues, preferably insertion of the sequence SSN, and preferably further comprising one or both of the substitutions I7Q and V3Y.

10

19. A BPN' like subtilase variant in which the ion-binding sites has been removed, wherein said variant comprises:

- 15 a) deletion of or in the region A194-L196 (Savinase in BPN' numbering) or a corresponding region in another BPN' like subtilase and insertion of three or more amino acid residues, preferably insertion of P209-P217 from JP170 or a corresponding region in another JP170 like subtilase and
- 20 deletion of or in the region L75-L82 (Savinase in BPN' numbering) or a corresponding region in said other BPN' like subtilase and insertion of one or more amino acid residues, preferably insertion of H83-Y92 from TY145 or a corresponding region in another TY145 like subtilase or
- b) deletion of or in the region A194-L196 (Savinase in BPN' numbering) or a corresponding region in another BPN' like subtilase and insertion of three or more amino acid residues, preferably insertion of P209-P217 from JP170 or a corresponding region in another JP170 like subtilase and
- 25 deletion of or in the L75-L82 (Savinase in BPN' numbering) or a corresponding region in said other BPN' like subtilase and insertion of one or more amino acid residues, preferably insertion of N79-K83 from JP170 or a corresponding region in another JP170 like subtilase.

- 30 20. A JP170 like subtilase variant comprising an alteration in one or more of the following positions:

13, 14, 15, 16, 17, 18,  
37, 38, 39, 40, 41, 42, 43,  
47, 48, 49, 50,

35 57, 58, 59,

96, 97, 98, 99, 100, 101, 102, 103,

131, 132, 133, 134,

152, 153

162, 163, 164, 165, 166,

5 188, 189, 190, 191, 192, 193, 194, 195,

210

234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246,

372, 373, 374, 375, 376, 377, 378,

387, 388, 389, 390, 391, 392,

10 406, 407 and

419.

21. A JP170 like subtilase variant comprising an alteration in one or more of the following positions:

15 37, 38, 39, 40, 41, 42,

57, 58, 59, 60,

66, 67,

98, 99, 100, 101, 102, 103,

107, 108, 109, 110, 111,

20 188, 189, 190, 191, 192, 193,

236, 237, 238, 239, 240,

326, 327, 328, 329, 330, 331, 332,

337, 338, 339, 340, 341, 342,

355, 356, 357, 358, 359, 360,

25 372, 373, 374, 375, 376, 377,

384, 385, 386, 387, 388,

404, 405, 406, 407, 408, 409, 410, 411.

22. A subtilase variant according to claim 21 comprising one or more of the modifications:

30 W240H,Y; G355A,S; S356T,N; T357N,Q,D,E,P; T358S; A359S,T,N,Q and S360T,N.

23. A variant subtilase comprising an alteration in one or more positions which are within a distance of 10Å from a Cl2 inhibitor which is bound to the active site of JP170, wherein the positions, as specified in SEQ ID NO:1 are:

29, 30, 31, 32, 64, 65, 66, 67, 68, 69, 70, 71, 72, 93, 96, 97, 98, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 113, 114, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 138, 139, 140, 141, 144, 157, 174, 180, 181, 182, 183, 191, 193, 194, 202, 203, 204, 205, 206, 207, 211, 223, 224, 225, 226, 234, 235, 236, 237, 238, 239, 240, 241, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258,

preferably comprising the substitution W129L.

24. A JP170 like subtilase variant comprising one or more disulfide bridges introduced by one or more of the following modifications: G21C/A86C, V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C, A27C/A122C, A45C/G78C, V72C/P258C, G78C/A229C, D98C/G104C, Q111C/Y147C, G135C/G167C, R142C/P354C, V144C/A178C, G182C/P217C, A183C/G223C, A195C/Y225C, F271C/P279C, A287C/A430C, A293C/S310C, E322C/S428C, S324C/A332C, S327C/P424C, D352C/N397C, G255C/T362C, G291C/S314C, A4C/P222C and A27C/V117C, wherein the positions correspond to the positions in SEQ ID NO:1

25. A JP170 like subtilase variant comprising an alteration in one or more of the positions N76, N316, L381, K246, K9, K313 and K83, preferably comprising one or more of the substitutions N79D, N316D, L381D, K246R, K9R, K313R and K83R of SEQ ID NO:1.

26. A JP170 like subtilase variant comprising an alteration in one or more of the positions 22, 44, 110, 139, 140, 166, 198, 201, 203, 231, 282, 356, 357 and 378, preferably comprising one or more of the substitutions: Q22P, E44P, L110P, T139P, D140P, S166P, I198P, V201P, Q203P, S231P, S282P, S356P, T357P and K378P.

27. A JP170 like subtilase variant comprising a deletion of the region 311-433, preferably deletion of positions 317-433 or 315-433, further comprising one or more of the substitutions L283N,Q; A290S,N and W306H,Y,K.

28. A subtilase variant according to claim 27, comprising

- a) deletion of positions 317-433 and the substitutions L283N, A290S and W306H, or
- b) deletion of region 315-433 and the substitutions L283N, A290S and W306H.

29. An isolated nucleic acid sequence comprising a nucleic acid sequence, which encodes for the subtilase variant defined or produced in any of the preceding claims.



30. An isolated nucleic acid sequence according to claim 29, wherein the nucleic acid sequence is selected from the group consisting of:

- 5 a) a nucleic acid sequence encoding an enzyme having at least 58% homology with the amino acid sequence shown in SEQ ID NO:1, and
- b) a nucleic acid sequence which hybridizes under low stringency conditions, preferably under medium stringency conditions, in particular under high stringency conditions, with a complementary strand of the nucleic acid sequence encoding an enzyme having at least 58% homology with the amino acid sequence shown in SEQ ID NO:1, or
- 10 c) a subsequence of any of a) or b) of at least 100 nucleotides.

31. An isolated nucleic acid construct comprising a nucleic acid sequence as defined in any of claims 29-30, operably linked to one or more control sequences capable of directing the expression of the polypeptide in a suitable expression host.

15

32. A recombinant host cell comprising the nucleic acid construct of claim 31.

33. A method for producing the variant defined in any of the preceding claims, the method comprising:

- 20 a) cultivating the recombinant host cell of claim 32 under conditions conducive to the production of the subtilase variant; and
- b) recovering the variant.

34. A detergent composition comprising a JP170 like subtilase variant or a BPN' like subtilase variant.

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35. Use of a JP170 like subtilase variant or a BPN' like subtilase variant in cleaning or washing applications.

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**ABSTRACT**

The present invention relates to methods for producing variants of a parent JP170 subtilase and of a parent BPN' subtilase and to JP170 and BPN' variants having altered properties as compared to the parent JP170/BPN' subtilase.

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Figure 1, Alignment of 3D sequences of protease JP170 (mature sequence from App. 1), SD-521 (aam50084 from EP 1209233) and protease Y (aay44619 from WO99/67370).

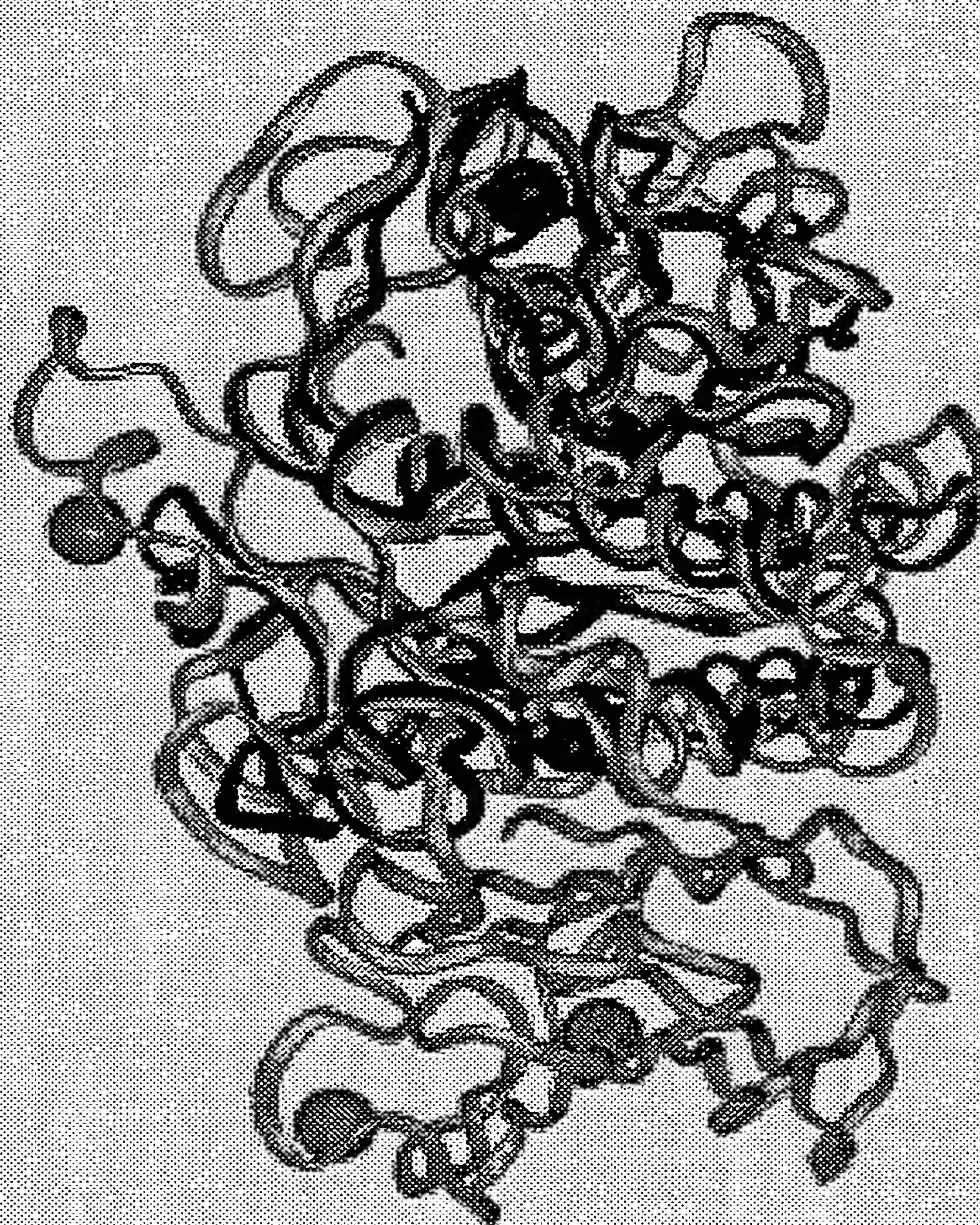
5	aam50084	1	NDVARGIVKA	DVAQNNGGLY	GQGQVVA	TGLDTGRNDS	SMHEAFRGKI	50
	aay44619		NDVARGIVKA	DVAQNNGGLY	GQGQLVA	TGLDTGRNDS	SMHEAFRGKI	
	JP170		NDVARGIVKA	DVAQNNFGLY	GQGQIVAVAD	TGLDTGRNDS	SMHEAFRGKI	
10	aam50084	51	TALYALGRTN	NANDPNGHGT	HVAGSVLGNA	LNKGMAPQAN	LVFQSIMDSS	100
	aay44619		TALYALGRTN	NASDPNGHGT	HVAGSVLGNA	LNKGMAPQAN	LVFQSIMDSS	
	JP170		TALYALGRTN	NANDPNGHGT	HVAGSVLGNA	TNKGMAPQAN	LVFQSIMDSG	
15	aam50084	101	GGLGGLPSNL	NTLFSQAWNA	GARIHTNSWG	APVNGAYTAN	SRQVDEYVRN	150
	aay44619		GGLGGLPSNL	NTLFSQAWNA	GARIHTNSWG	APVNGAYTAN	SRQVDEYVRN	
	JP170		GGLGGLPANL	QTLFSQAYSA	GARIHTNSWG	APVNGAYTTD	SRNVDDYVRK	
20	aam50084	151	NDMTVLFAAG	NEGPNSGTIS	APGTAKNAIT	VGATENYRPS	FGSLADNPNH	200
	aay44619		NDMTVLFAAG	NEGPNSGTIS	APGTAKNAIT	VGATENYRPS	FGSIADNPNH	
	JP170		NDMTILFAAG	NEGPGSGTIS	APGTAKNAIT	VGATENLRPS	FGSYADNINH	
25	aam50084	201	IAQFSSRGAT	RDGRIKPDVT	APGTFILSAR	SSLAPDSSFW	ANYNSKYAYM	250
	aay44619		IAQFSSRGAT	RDGRIKPDVT	APGTFILSAR	SSLAPDSSFW	ANYNSKYAYM	
	JP170		VAQFSSRGFT	RDGRIKPDVM	APGTYILSAR	SSLAPDSSFW	ANHDSKYAYM	
30	aam50084	251	GGTSMATPIV	AGNVAQLREH	FIKNRGITPK	PSLIKAALIA	GATDVGLGYP	300
	aay44619		GGTSMATPIV	AGNVAQLREH	FIKNRGITPK	PSLIKAALIA	GATDVGLGYP	
	JP170		GGTSMATPIV	AGNVAQLREH	FVKNRGVTPK	PSLLKAALIA	GAADVGLGFP	
35	aam50084	301	SGDQGWGRVT	LDKSLNVAYV	NEATALATGQ	KATYSFQAQA	GKPLKISLVW	350
	aay44619		SGDQGWGRVT	LDKSLNVAYV	NEATALATGQ	KATYSFQAQA	GKPLKISLVW	
	JP170		NGNQGWGRVT	LDKSLNVAFV	NETSPLSTSQ	KATYSFTAQA	GKPLKISLVW	
40	aam50084	351	TDAPGSTTAS	YTLVNDLIDL	ITAPNGQKYV	GNDFSYPYDN	NWDGRNNVEN	400
	aay44619		TDAPGSTTAS	YTLVNDLIDL	ITAPNGQKYV	GNDFSYPYDN	NWDGRNNVEN	
	JP170		SDAPGSTTAS	LTLVNDLIDL	ITAPNGTKYV	GNDFTAPYDN	NWDGRNNVEN	
45	aam50084	401	VFINAPQSGT	YTIEVQAYNV	PSGPQRFSLA	IVH		433
	aay44619		VFINAPQSGT	YIIEVQAYNV	PSGPQRFSLA	IVH		
	JP170		VFINAPQSGT	YTVEVQAYNV	PVSPQTFSLA	IVH		

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Figure 2, Superposition of JP170 and Savinase 3D structures, with indication of calcium binding sites. JP170: light structure and three ion-binding sites. Savinase: dark structure and two ion-binding sites.





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Figure 3, Matrix of homology between subtilases pertaining to the JP170, TY145 and BPN' subgroups. The sequences are identified by sequence database accession numbers:

- 00: aam50084; Subtilase derived from *Bacillus* sp. strain SD-521
- 5 0: aaw89547; Subtilase derived from *Bacillus* sp. JP170
- 1: q45681; Subtilase derived from *B. subtilis* (BSTA41)
- 2: p28842; Psychrophilic subtilisin derived from Antarctic *Bacillus* strain (BSTA39)
- 3: abb77095; Subtilase derived from *Bacillus* sp. (TY145)
- 4: p00783; Subtilase derived from *Bacillus subtilis* var. *amylosacchariticus* (BSAMY)
- 10 5: p29142; Subtilase derived from *Bacillus stearothermophilus* (BSSJ)
- 6: p35835; Subtilase derived from *Bacillus subtilis* var. *natto*. (BSNAT)
- 7: p07518; Subtilase derived from *Bacillus pumilus* (*B. mesentericus*) (BPMES)
- 8: p00782; Subtilase derived from *Bacillus amyloliquefaciens* (BPN')
- 9: p00780; Subtilase derived from *Bacillus licheniformis* (BLSCAR)
- 15 10: p41363; Subtilase derived from *Bacillus halodurans* (BHSAH)
- 11: aaw62222; Subtilase derived from *Bacillus lentus* (BLS147)
- 12: p29600; Subtilase derived from *Bacillus lentus* (BLSAVI, BLS309)
- 13: p27693; Subtilase derived from *Bacillus alcalophilus* (BAALKP)
- 14: q99405; Subtilase derived from *Bacillus* sp. strain KSM-K16 (BSKSMK)
- 20 15: p29599; Subtilase derived from *Bacillus lentus* (BLSUBL).

	00	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
00 aam50084	100	94	53	53	51	53	53	52	52	53	55	52	52	51	51	51	50
0 aaw89547		100	52	53	53	51	51	49	50	51	51	50	54	54	53	54	54
25 1 q45681			100	93	76	51	50	51	55	52	54	58	58	59	57	60	60
2 p28842				100	75	52	52	52	56	53	55	58	58	61	58	62	61
3 abb77095					100	60	60	60	58	60	62	58	57	59	59	62	59
4 p00783						100	99	99	97	91	76	63	69	74	66	74	74
5 p29142							100	99	97	90	76	69	74	66	74	74	56
30 6 p35835								100	98	91	77	63	69	74	66	74	74
7 p07518									100	88	79	69	67	74	74	74	74
8 p00782										100	77	66	71	74	67	74	74
9 p00780											100	64	69	74	67	73	73
10 p41363												100	99	76	72	76	76
35 11 aaw62222													100	76	76	76	76
12 p29600														100	99	99	99
13 p27693															100	99	99
14 q99405																100	98
15 p29599																	100

40



10321 SEQ list.ST25  
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21 MRS. 2003

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35 40 45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Asn Asp  
50 55 60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala  
65 70 75 80

Thr Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile  
85 90 95

Met Asp Ser Gly Gly Gly Leu Gly Gly Leu Pro Ala Asn Leu Gln Thr  
100 105 110

Leu Phe Ser Gln Ala Tyr Ser Ala Gly Ala Arg Ile His Thr Asn Ser  
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Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Thr Asp Ser Arg Asn Val  
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Asn Glu Gly Pro Gly Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys  
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Ser Tyr Ala Asp Asn Ile Asn His Val Ala Gln Phe Ser Ser Arg Gly  
195 200 205

Pro Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Met Ala Pro Gly Thr  
210 215 220

Tyr Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp  
225 230 235 240

Ala Asn His Asp Ser Lys Tyr Ala Tyr Met Gly Gly Thr Ser Met Ala  
245 250 255

Thr Pro Ile Val Ala Gly Asn Val Ala Gln Leu Arg Glu His Phe Val  
260 265 270

Lys Asn Arg Gly Val Thr Pro Lys Pro Ser Leu Leu Lys Ala Ala Leu  
275 280 285

Ile Ala Gly Ala Ala Asp Val Gly Leu Gly Phe Pro Asn Gly Asn Gln  
290 295 300

Gly Trp Gly Arg Val Thr Leu Asp Lys Ser Leu Asn Val Ala Phe Val  
305 310 315 320

Asn Glu Thr Ser Pro Leu Ser Thr Ser Gln Lys Ala Thr Tyr Ser Phe  
325 330 335

Thr Ala Gln Ala Gly Lys Pro Leu Lys Ile Ser Leu Val Trp Ser Asp  
340 345 350

Ala Pro Gly Ser Thr Thr Ala Ser Leu Thr Leu Val Asn Asp Leu Asp  
355 360 365

Leu Val Ile Thr Ala Pro Asn Gly Thr Lys Tyr Val Gly Asn Asp Phe  
370 375 380

Thr Ala Pro Tyr Asp Asn Asn Trp Asp Gly Arg Asn Asn Val Glu Asn  
385 390 395 400

Val Phe Ile Asn Ala Pro Gln Ser Gly Thr Tyr Thr Val Glu Val Gln  
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Ala Tyr Asn Val Pro Val Ser Pro Gln Thr Phe Ser Leu Ala Ile Val  
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His

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 20 25 30

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 35 40 45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Ser Asp  
 50 55 60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala  
 65 70 75 80

Leu Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile  
 85 90 95

Met Asp Ser Ser Gly Gly Leu Gly Gly Leu Pro Ser Asn Leu Asn Thr  
 100 105 110

Leu Phe Ser Gln Ala Trp Asn Ala Gly Ala Arg Ile His Thr Asn Ser  
 115 120 125

Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Ala Asn Ser Arg Gln Val  
 130 135 140

Asp Glu Tyr Val Arg Asn Asn Asp Met Thr Val Leu Phe Ala Ala Gly  
 145 150 155 160

Asn Glu Gly Pro Asn Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys  
 165 170 175

Asn Ala Ile Thr Val Gly Ala Thr Glu Asn Tyr Arg Pro Ser Phe Gly  
 180 185 190

Ser Ile Ala Asp Asn Pro Asn His Ile Ala Gln Phe Ser Ser Arg Gly  
 195 200 205

Ala Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Thr Ala Pro Gly Thr  
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10321 SEQ list.ST25

Phe Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp  
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Ala Asn Tyr Asn Ser Lys Tyr Ala Tyr Met Gly Gly Thr Ser Met Ala  
 245 250 255

Thr Pro Ile Val Ala Gly Asn Val Ala Gln Leu Arg Glu His Phe Ile  
 260 265 270

Lys Asn Arg Gly Ile Thr Pro Lys Pro Ser Leu Ile Lys Ala Ala Leu  
 275 280 285

Ile Ala Gly Ala Thr Asp Val Gly Leu Gly Tyr Pro Ser Gly Asp Gln  
 290 295 300

Gly Trp Gly Arg Val Thr Leu Asp Lys Ser Leu Asn Val Ala Tyr Val  
 305 310 315 320

Asn Glu Ala Thr Ala Leu Ala Thr Gly Gln Lys Ala Thr Tyr Ser Phe  
 325 330 335

Gln Ala Gln Ala Gly Lys Pro Leu Lys Ile Ser Leu Val Trp Thr Asp  
 340 345 350

Ala Pro Gly Ser Thr Thr Ala Ser Tyr Thr Leu Val Asn Asp Leu Asp  
 355 360 365

Leu Val Ile Thr Ala Pro Asn Gly Gln Lys Tyr Val Gly Asn Asp Phe  
 370 375 380

Ser Tyr Pro Tyr Asp Asn Asn Trp Asp Gly Arg Asn Asn Val Glu Asn  
 385 390 395 400

Val Phe Ile Asn Ala Pro Gln Ser Gly Thr Tyr Ile Ile Glu Val Gln  
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Ala Tyr Asn Val Pro Ser Gly Pro Gln Arg Phe Ser Leu Ala Ile Val  
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His

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## 10321 SEQ list.ST25

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Tyr Gly Leu Tyr Gly Gln Gly Gln Val Val Ala Val Ala Asp Thr Gly  
20 25 30

Leu Asp Thr Gly Arg Asn Asp Ser Ser Met His Glu Ala Phe Arg Gly  
35 40 45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Asn Asp  
50 55 60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala  
65 70 75 80

Leu Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile  
85 90 95

Met Asp Ser Ser Gly Gly Leu Gly Gly Leu Pro Ser Asn Leu Asn Thr  
100 105 110

Leu Phe Ser Gln Ala Trp Asn Ala Gly Ala Arg Ile His Thr Asn Ser  
115 120 125

Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Ala Asn Ser Arg Gln Val  
130 135 140

Asp Glu Tyr Val Arg Asn Asn Asp Met Thr Val Leu Phe Ala Ala Gly  
145 150 155 160

Asn Glu Gly Pro Asn Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys  
165 170 175

Asn Ala Ile Thr Val Gly Ala Thr Glu Asn Tyr Arg Pro Ser Phe Gly  
180 185 190

Ser Leu Ala Asp Asn Pro Asn His Ile Ala Gln Phe Ser Ser Arg Gly  
195 200 205

Ala Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Thr Ala Pro Gly Thr  
210 215 220

Phe Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp  
225 230 235 240

Ala Asn Tyr Asn Ser Lys Tyr Ala Tyr Met Gly Gly Thr Ser Met Ala  
245 250 255

Thr Pro Ile Val Ala Gly Asn Val Ala Gln Leu Arg Glu His Phe Ile



Lys Asn Arg Gly Ile Thr Pro Lys Pro Ser Leu Ile Lys Ala Ala Leu  
275 280 285

Ile Ala Gly Ala Thr Asp Val Gly Leu Gly Tyr Pro Ser Gly Asp Gln  
290 295 300

Gly Trp Gly Arg Val Thr Leu Asp Lys Ser Leu Asn Val Ala Tyr Val  
305 310 315 320

Asn Glu Ala Thr Ala Leu Ala Thr Gly Gln Lys Ala Thr Tyr Ser Phe  
325 330 335

Gln Ala Gln Ala Gly Lys Pro Leu Lys Ile Ser Leu Val Trp Thr Asp  
340 345 350

Ala Pro Gly Ser Thr Thr Ala Ser Tyr Thr Leu Val Asn Asp Leu Asp  
355 360 365

Leu Val Ile Thr Ala Pro Asn Gly Gln Lys Tyr Val Gly Asn Asp Phe  
370 375 380

Ser Tyr Pro Tyr Asp Asn Asn Trp Asp Gly Arg Asn Asn Val Glu Asn  
385 390 395 400

Val Phe Ile Asn Ala Pro Gln Ser Gly Thr Tyr Thr Ile Glu Val Gln  
405 410 415

Ala Tyr Asn Val Pro Ser Gly Pro Gln Arg Phe Ser Leu Ala Ile Val  
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His

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10321 SEQ list.ST25

His Ser Gln Gly Tyr Thr Gly Ser Asn Val Lys Val Ala Val Ile Asp  
20 25 30

Ser Gly Ile Asp Ser Ser His Pro Asp Leu Lys Val Ala Gly Gly Ala  
35 40 45

Ser Met Val Pro Ser Glu Thr Asn Pro Phe Gln Asp Asn Asn Ser His  
50 55 60

Gly Thr His Val Ala Gly Thr Val Ala Ala Leu Asn Asn Ser Ile Gly  
65 70 75 80

Val Leu Gly Val Ala Pro Ser Ala Ser Leu Tyr Ala Val Lys Val Leu  
85 90 95

Gly Ala Asp Gly Ser Gly Gln Tyr Ser Trp Ile Ile Asn Gly Ile Glu  
100 105 110

Trp Ala Ile Ala Asn Asn Met Asp Val Ile Asn Met Ser Leu Gly Gly  
115 120 125

Pro Ser Gly Ser Ala Ala Leu Lys Ala Ala Val Asp Lys Ala Val Ala  
130 135 140

Ser Gly Val Val Val Val Ala Ala Ala Gly Asn Glu Gly Thr Ser Gly  
145 150 155 160

Ser Ser Ser Thr Val Gly Tyr Pro Gly Lys Tyr Pro Ser Val Ile Ala  
165 170 175

Val Gly Ala Val Asp Ser Ser Asn Gln Arg Ala Ser Phe Ser Ser Val  
180 185 190

Gly Pro Glu Leu Asp Val Met Ala Pro Gly Val Ser Ile Gln Ser Thr  
195 200 205

Leu Pro Gly Asn Lys Tyr Gly Ala Tyr Asn Gly Thr Ser Met Ala Ser  
210 215 220

Pro His Val Ala Gly Ala Ala Ala Leu Ile Leu Ser Lys His Pro Asn  
225 230 235 240

Trp Thr Asn Thr Gln Val Arg Ser Ser Leu Glu Asn Thr Thr Thr Lys  
245 250 255

Leu Gly Asp Ser Phe Tyr Tyr Gly Lys Gly Leu Ile Asn Val Gln Ala  
260 265 270

Ala Ala Gln  
275

21 MRS. 2003

## APPENDIX 1

REMARK Complex of JP170 and CI2A inhibitor  
REMARK Contents of asymmetric unit subtilisin 2x (433 a.a. x 2)  
REMARK CI2A inhibitor 2x (a.a. 16 - 83 and 21 - 83)  
REMARK small peptide (autodigestion product, a.a. KPSLL, 280 - 284)  
REMARK Ca ions 6x, H2O 1115 x  
REMARK  
REMARK Crystallization conditions: (AMB) Hanging drop vapour diffusion  
REMARK method where the drop consists of 2 µl of 15 - 20 mg.ml<sup>-1</sup>  
REMARK protein concentration, 10 mM Na cacodylate - HCl buffer, pH 6.5  
REMARK and 1 µl of the well solution, 20% w/v PEG 4000, 0.1 M Hepes  
REMARK buffer, pH 7.5, 10% v/v isopropanol.

HEADER ----- XX-XXX-XX      XXXX  
COMPND ----  
REMARK 3  
REMARK 3 REFINEMENT.  
REMARK 3    PROGRAM        : REFMAC 5.1.24  
REMARK 3    AUTHORS      : MURSHUDOV,VAGIN,DODSON  
REMARK 3  
REMARK 3       REFINEMENT TARGET : MAXIMUM LIKELIHOOD  
REMARK 3  
REMARK 3 DATA USED IN REFINEMENT.  
REMARK 3    RESOLUTION RANGE HIGH (ANGSTROMS) :    1.90  
REMARK 3    RESOLUTION RANGE LOW    (ANGSTROMS) :    19.96  
REMARK 3    DATA CUTOFF                    (SIGMA(F)) : NONE  
REMARK 3    COMPLETENESS FOR RANGE                    (%) :    76.65  
REMARK 3    NUMBER OF REFLECTIONS                    :    59444  
REMARK 3  
REMARK 3 FIT TO DATA USED IN REFINEMENT.  
REMARK 3    CROSS-VALIDATION METHOD                    : NULL  
REMARK 3    FREE R VALUE TEST SET SELECTION           : NULL  
REMARK 3    R VALUE                    (WORKING + TEST SET) : 0.12256  
REMARK 3    R VALUE                    (WORKING SET)       : 0.12256  
REMARK 3    FREE R VALUE                                : NULL  
REMARK 3    FREE R VALUE TEST SET SIZE                (%) : NULL  
REMARK 3    FREE R VALUE TEST SET COUNT                : NULL  
REMARK 3  
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.  
REMARK 3    TOTAL NUMBER OF BINS USED                    :       20  
REMARK 3    BIN RESOLUTION RANGE HIGH                    :    1.901  
REMARK 3    BIN RESOLUTION RANGE LOW                    :    1.950  
REMARK 3    REFLECTION IN BIN                    (WORKING SET) :       940  
REMARK 3    BIN R VALUE                    (WORKING SET) :    0.149  
REMARK 3    BIN FREE R VALUE SET COUNT                    :       0  
REMARK 3    BIN FREE R VALUE                                : -999.000  
REMARK 3  
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.  
REMARK 3    ALL ATOMS                                :    8694  
REMARK 3  
REMARK 3 B VALUES.  
REMARK 3    FROM WILSON PLOT                                (A\*\*2) : NULL  
REMARK 3    MEAN B VALUE                    (OVERALL, A\*\*2) :    16.479  
REMARK 3    OVERALL ANISOTROPIC B VALUE.  
REMARK 3    B11 (A\*\*2) :       0.05  
REMARK 3    B22 (A\*\*2) :       0.06  
REMARK 3    B33 (A\*\*2) :      -0.11  
REMARK 3    B12 (A\*\*2) :       0.00

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REMARK 3      B13 (A**2) :      0.00
REMARK 3      B23 (A**2) :      0.00
REMARK 3
REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK 3      ESU BASED ON R VALUE (A) :      0.151
REMARK 3      ESU BASED ON FREE R VALUE (A) : NULL
REMARK 3      ESU BASED ON MAXIMUM LIKELIHOOD (A) :      0.052
REMARK 3      ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) :      1.828
REMARK 3
REMARK 3 CORRELATION COEFFICIENTS.
REMARK 3      CORRELATION COEFFICIENT FO-FC :      0.969
REMARK 3      CORRELATION COEFFICIENT FO-FC FREE : NULL
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES          COUNT      RMS      WEIGHT
REMARK 3      BOND LENGTHS REFINED ATOMS (A) : 7733 ; 0.014 ; 0.021
REMARK 3      BOND LENGTHS OTHERS (A) : 6857 ; 0.001 ; 0.020
REMARK 3      BOND ANGLES REFINED ATOMS (DEGREES) : 10540 ; 1.478 ; 1.936
REMARK 3      BOND ANGLES OTHERS (DEGREES) : 15972 ; 0.815 ; 3.000
REMARK 3      TORSION ANGLES, PERIOD 1 (DEGREES) : 997 ; 15.784 ; 5.000
REMARK 3      CHIRAL-CENTER RESTRAINTS (A**3) : 1197 ; 0.106 ; 0.200
REMARK 3      GENERAL PLANES REFINED ATOMS (A) : 8819 ; 0.007 ; 0.020
REMARK 3      GENERAL PLANES OTHERS (A) : 1500 ; 0.008 ; 0.020
REMARK 3      NON-BONDED CONTACTS REFINED ATOMS (A) : 1552 ; 0.221 ; 0.300
REMARK 3      NON-BONDED CONTACTS OTHERS (A) : 8282 ; 0.265 ; 0.300
REMARK 3      NON-BONDED TORSION OTHERS (A) : 4417 ; 0.089 ; 0.500
REMARK 3      H-BOND (X...Y) REFINED ATOMS (A) : 1391 ; 0.198 ; 0.500
REMARK 3      POTENTIAL METAL-ION REFINED ATOMS (A) : 25 ; 0.145 ; 0.500
REMARK 3      SYMMETRY VDW REFINED ATOMS (A) : 10 ; 0.129 ; 0.300
REMARK 3      SYMMETRY VDW OTHERS (A) : 57 ; 0.268 ; 0.300
REMARK 3      SYMMETRY H-BOND REFINED ATOMS (A) : 87 ; 0.272 ; 0.500
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS.          COUNT      RMS      WEIGHT
REMARK 3      MAIN-CHAIN BOND REFINED ATOMS (A**2) : 4985 ; 0.697 ; 1.500
REMARK 3      MAIN-CHAIN ANGLE REFINED ATOMS (A**2) : 8031 ; 1.205 ; 2.000
REMARK 3      SIDE-CHAIN BOND REFINED ATOMS (A**2) : 2746 ; 1.963 ; 3.000
REMARK 3      SIDE-CHAIN ANGLE REFINED ATOMS (A**2) : 2509 ; 3.180 ; 4.500
REMARK 3
REMARK 3 NCS RESTRAINTS STATISTICS
REMARK 3      NUMBER OF NCS GROUPS : NULL
REMARK 3
REMARK 3
REMARK 3 TLS DETAILS
REMARK 3      NUMBER OF TLS GROUPS : NULL
REMARK 3
REMARK 3
REMARK 3 BULK SOLVENT MODELLING.
REMARK 3      METHOD USED : BABINET MODEL WITH MASK
REMARK 3      PARAMETERS FOR MASK CALCULATION
REMARK 3      VDW PROBE RADIUS : 1.40
REMARK 3      ION PROBE RADIUS : 0.80
REMARK 3      SHRINKAGE RADIUS : 0.80
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS:
REMARK 3      HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK 3
CISPEP 1 GLY A 163      PRO A 164      0.00
CISPEP 2 ALA A 171      PRO A 172      0.00
CISPEP 3 PHE A 191      GLY A 192      0.00

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CISPEP	4	ASN	A	199	HIS	A	200		0.00		
CISPEP	5	GLY	A	208	PRO	A	209		0.00		
CISPEP	6	LYS	A	216	PRO	A	217		0.00		
CISPEP	7	ASP	A	236	SER	A	237		0.00		
CISPEP	8	ASP	A	244	SER	A	245		0.00		
CISPEP	9	PHE	A	299	PRO	A	300		0.00		
CISPEP	10	SER	A	327	THR	A	328		0.00		
CISPEP	11	ALA	A	386	PRO	A	387		0.00		
CISPEP	12	GLU	A	414	VAL	A	415		0.00		
CISPEP	13	GLY	A	423	PRO	A	424		0.00		
LINK				ASN B 316				LYS B 318		gap	
LINK				GLU B 330				ALA B 332		gap	
LINK				LEU B 337				LYS B 340		gap	
LINK				GLU D 330				ALA D 332		gap	
LINK				LEU D 337				LYS D 340		gap	
CISPEP	14	GLY	C	163	PRO	C	164		0.00		
CISPEP	15	ALA	C	171	PRO	C	172		0.00		
CISPEP	16	PHE	C	191	GLY	C	192		0.00		
CISPEP	17	ASN	C	199	HIS	C	200		0.00		
CISPEP	18	GLY	C	208	PRO	C	209		0.00		
CISPEP	19	LYS	C	216	PRO	C	217		0.00		
CISPEP	20	ASP	C	236	SER	C	237		0.00		
CISPEP	21	ASP	C	244	SER	C	245		0.00		
CISPEP	22	PHE	C	299	PRO	C	300		0.00		
CISPEP	23	SER	C	327	THR	C	328		0.00		
CISPEP	24	ALA	C	386	PRO	C	387		0.00		
CISPEP	25	GLU	C	414	VAL	C	415		0.00		
CISPEP	26	GLY	C	423	PRO	C	424		0.00		
CRYST1	58.387	151.411		64.054	90.00	117.11	90.00	P 1 21 1			
SCALE1	0.017127	0.000000		0.008768			0.000000				
SCALE2	0.000000	0.006605		0.000000			0.000000				
SCALE3	0.000000	0.000000		0.017539			0.000000				
HETATM	1	N	ASN	A	1	18.066	20.808	-3.996	1.00	14.87	A N
HETATM	2	C9	ASN	A	1	18.461	22.053	-3.689	1.00	14.47	A C
HETATM	3	O10	ASN	A	1	19.168	22.251	-2.661	1.00	13.33	A O
HETATM	4	O11	ASN	A	1	18.108	23.029	-4.423	1.00	14.69	A O
HETATM	5	CA	ASN	A	1	18.499	19.635	-3.189	1.00	14.35	A C
HETATM	6	CB	ASN	A	1	18.164	18.329	-3.883	1.00	14.69	A C
HETATM	7	CG	ASN	A	1	16.670	18.063	-4.031	1.00	14.08	A C
HETATM	8	ND2	ASN	A	1	16.271	17.100	-5.019	1.00	12.20	A N
HETATM	9	OD1	ASN	A	1	15.768	18.701	-3.206	1.00	14.76	A O
HETATM	10	C	ASN	A	1	19.990	19.659	-2.890	1.00	14.84	A C
HETATM	11	O	ASN	A	1	20.353	19.313	-1.601	1.00	14.20	A O
ATOM	12	N	ASP	A	2	20.881	19.935	-3.834	1.00	15.84	A N
ATOM	13	CA	ASP	A	2	22.306	19.835	-3.520	1.00	16.82	A C
ATOM	14	CB	ASP	A	2	23.178	20.088	-4.763	1.00	17.53	A C
ATOM	15	CG	ASP	A	2	23.121	18.947	-5.783	1.00	18.18	A C
ATOM	16	OD1	ASP	A	2	22.652	17.811	-5.493	1.00	20.58	A O
ATOM	17	OD2	ASP	A	2	23.544	19.106	-6.931	1.00	22.02	A O
ATOM	18	C	ASP	A	2	22.712	20.816	-2.413	1.00	17.23	A C
ATOM	19	O	ASP	A	2	23.671	20.562	-1.703	1.00	18.17	A O
ATOM	20	N	VAL	A	3	22.018	21.952	-2.304	1.00	17.05	A N
ATOM	21	CA	VAL	A	3	22.374	22.945	-1.311	1.00	16.07	A C
ATOM	22	CB	VAL	A	3	21.974	24.356	-1.701	1.00	16.60	A C
ATOM	23	CG1	VAL	A	3	22.327	25.323	-0.560	1.00	16.25	A C
ATOM	24	CG2	VAL	A	3	22.676	24.770	-3.003	1.00	18.81	A C
ATOM	25	C	VAL	A	3	21.749	22.565	0.033	1.00	15.65	A C
ATOM	26	O	VAL	A	3	22.431	22.603	1.090	1.00	14.41	A O



ATOM	27	N	ALA	A	4	20.497	22.119	-0.012	1.00	13.75	A	N
ATOM	28	CA	ALA	A	4	19.824	21.664	1.196	1.00	14.03	A	C
ATOM	29	CB	ALA	A	4	18.388	21.260	0.881	1.00	13.78	A	C
ATOM	30	C	ALA	A	4	20.544	20.512	1.876	1.00	14.28	A	C
ATOM	31	O	ALA	A	4	20.548	20.406	3.110	1.00	14.07	A	O
ATOM	32	N	ARG	A	5	21.093	19.617	1.064	1.00	13.74	A	N
ATOM	33	CA	ARG	A	5	21.807	18.445	1.553	1.00	14.95	A	C
ATOM	34	CB	ARG	A	5	22.395	17.709	0.349	1.00	15.61	A	C
ATOM	35	CG	ARG	A	5	23.452	16.639	0.631	1.00	17.28	A	C
ATOM	36	CD	ARG	A	5	23.873	15.945	-0.672	1.00	20.73	A	C
ATOM	37	NE	ARG	A	5	24.802	14.852	-0.459	1.00	21.95	A	N
ATOM	38	CZ	ARG	A	5	26.128	14.986	-0.513	1.00	24.69	A	C
ATOM	39	NH1	ARG	A	5	26.687	16.173	-0.793	1.00	25.62	A	N
ATOM	40	NH2	ARG	A	5	26.898	13.933	-0.290	1.00	22.96	A	N
ATOM	41	C	ARG	A	5	22.918	18.840	2.515	1.00	14.83	A	C
ATOM	42	O	ARG	A	5	23.135	18.195	3.546	1.00	14.86	A	O
ATOM	43	N	GLY	A	6	23.641	19.897	2.166	1.00	15.33	A	N
ATOM	44	CA	GLY	A	6	24.677	20.416	3.044	1.00	15.34	A	C
ATOM	45	C	GLY	A	6	24.094	21.124	4.257	1.00	15.01	A	C
ATOM	46	O	GLY	A	6	24.609	20.980	5.362	1.00	14.62	A	O
ATOM	47	N	ILE	A	7	23.018	21.879	4.062	1.00	14.44	A	N
ATOM	48	CA	ILE	A	7	22.411	22.613	5.168	1.00	13.98	A	C
ATOM	49	CB	ILE	A	7	21.266	23.505	4.698	1.00	13.68	A	C
ATOM	50	CG1	ILE	A	7	21.813	24.676	3.864	1.00	13.35	A	C
ATOM	51	CD1	ILE	A	7	20.794	25.294	2.972	1.00	14.08	A	C
ATOM	52	CG2	ILE	A	7	20.511	24.072	5.873	1.00	12.51	A	C
ATOM	53	C	ILE	A	7	21.970	21.664	6.305	1.00	15.04	A	C
ATOM	54	O	ILE	A	7	22.273	21.906	7.469	1.00	13.35	A	O
ATOM	55	N	VAL	A	8	21.320	20.558	5.952	1.00	15.03	A	N
ATOM	56	CA	VAL	A	8	20.795	19.628	6.969	1.00	14.89	A	C
ATOM	57	CB	VAL	A	8	19.419	19.047	6.545	1.00	14.63	A	C
ATOM	58	CG1	VAL	A	8	18.472	20.135	6.246	1.00	14.63	A	C
ATOM	59	CG2	VAL	A	8	19.526	18.151	5.333	1.00	15.54	A	C
ATOM	60	C	VAL	A	8	21.770	18.511	7.356	1.00	14.75	A	C
ATOM	61	O	VAL	A	8	21.438	17.645	8.168	1.00	15.23	A	O
ATOM	62	N	LYS	A	9	22.983	18.568	6.804	1.00	14.02	A	N
ATOM	63	CA	LYS	A	9	24.061	17.627	7.118	1.00	14.55	A	C
ATOM	64	CB	LYS	A	9	24.374	17.560	8.621	1.00	15.28	A	C
ATOM	65	CG	LYS	A	9	24.553	18.888	9.299	1.00	18.34	A	C
ATOM	66	CD	LYS	A	9	25.757	19.608	8.810	1.00	23.66	A	C
ATOM	67	CE	LYS	A	9	26.025	20.904	9.618	1.00	28.33	A	C
ATOM	68	NZ	LYS	A	9	27.283	21.559	9.079	1.00	31.91	A	N
ATOM	69	C	LYS	A	9	23.798	16.226	6.616	1.00	13.77	A	C
ATOM	70	O	LYS	A	9	24.391	15.256	7.132	1.00	13.96	A	O
ATOM	71	N	ALA	A	10	22.979	16.109	5.569	1.00	13.98	A	N
ATOM	72	CA	ALA	A	10	22.816	14.830	4.886	1.00	14.34	A	C
ATOM	73	CB	ALA	A	10	21.649	14.866	3.848	1.00	14.47	A	C
ATOM	74	C	ALA	A	10	24.141	14.437	4.205	1.00	14.55	A	C
ATOM	75	O	ALA	A	10	24.409	13.264	4.015	1.00	13.73	A	O
ATOM	76	N	ASP	A	11	24.967	15.423	3.860	1.00	16.04	A	N
ATOM	77	CA	ASP	A	11	26.278	15.153	3.265	1.00	17.11	A	C
ATOM	78	CB	ASP	A	11	26.899	16.419	2.667	1.00	17.53	A	C
ATOM	79	CG	ASP	A	11	27.059	17.547	3.680	1.00	19.89	A	C
ATOM	80	OD1	ASP	A	11	27.845	18.461	3.375	1.00	23.81	A	O
ATOM	81	OD2	ASP	A	11	26.434	17.635	4.773	1.00	20.19	A	O
ATOM	82	C	ASP	A	11	27.219	14.489	4.285	1.00	17.57	A	C
ATOM	83	O	ASP	A	11	27.941	13.540	3.947	1.00	17.08	A	O
ATOM	84	N	VAL	A	12	27.153	14.945	5.528	1.00	17.31	A	N

ATOM	85	CA	VAL	A	12	27.926	14.338	6.607	1.00	17.86	A	C
ATOM	86	CB	VAL	A	12	27.850	15.193	7.893	1.00	18.12	A	C
ATOM	87	CG1	VAL	A	12	28.577	14.533	9.081	1.00	18.00	A	C
ATOM	88	CG2	VAL	A	12	28.385	16.633	7.631	1.00	19.36	A	C
ATOM	89	C	VAL	A	12	27.428	12.898	6.835	1.00	18.14	A	C
ATOM	90	O	VAL	A	12	28.233	11.956	6.925	1.00	18.38	A	O
ATOM	91	N	ALA	A	13	26.117	12.696	6.870	1.00	17.13	A	N
ATOM	92	CA	ALA	A	13	25.572	11.353	7.076	1.00	17.08	A	C
ATOM	93	CB	ALA	A	13	24.070	11.400	7.101	1.00	17.00	A	C
ATOM	94	C	ALA	A	13	26.044	10.394	5.981	1.00	17.57	A	C
ATOM	95	O	ALA	A	13	26.472	9.237	6.254	1.00	16.79	A	O
ATOM	96	N	GLN	A	14	25.934	10.862	4.740	1.00	17.24	A	N
ATOM	97	CA	GLN	A	14	26.420	10.107	3.582	1.00	17.55	A	C
ATOM	98	CB	GLN	A	14	25.972	10.825	2.309	1.00	17.74	A	C
ATOM	99	CG	GLN	A	14	24.485	10.673	2.031	1.00	17.61	A	C
ATOM	100	CD	GLN	A	14	23.995	11.535	0.887	1.00	20.02	A	C
ATOM	101	OE1	GLN	A	14	24.788	11.949	0.028	1.00	19.60	A	O
ATOM	102	NE2	GLN	A	14	22.679	11.789	0.850	1.00	19.07	A	N
ATOM	103	C	GLN	A	14	27.949	9.876	3.576	1.00	18.95	A	C
ATOM	104	O	GLN	A	14	28.413	8.729	3.489	1.00	18.61	A	O
ATOM	105	N	ASN	A	15	28.730	10.950	3.658	1.00	19.73	A	N
ATOM	106	CA	ASN	A	15	30.185	10.847	3.469	1.00	20.71	A	C
ATOM	107	CB	ASN	A	15	30.828	12.222	3.244	1.00	20.45	A	C
ATOM	108	CG	ASN	A	15	30.404	12.869	1.959	1.00	22.21	A	C
ATOM	109	OD1	ASN	A	15	30.098	12.201	0.976	1.00	25.39	A	O
ATOM	110	ND2	ASN	A	15	30.390	14.182	1.953	1.00	23.97	A	N
ATOM	111	C	ASN	A	15	30.865	10.185	4.653	1.00	20.49	A	C
ATOM	112	O	ASN	A	15	31.705	9.362	4.469	1.00	21.06	A	O
ATOM	113	N	ASN	A	16	30.495	10.559	5.869	1.00	21.00	A	N
ATOM	114	CA	ASN	A	16	31.148	10.056	7.073	1.00	21.90	A	C
ATOM	115	CB	ASN	A	16	31.205	11.146	8.136	1.00	22.29	A	C
ATOM	116	CG	ASN	A	16	32.100	12.313	7.751	1.00	26.21	A	C
ATOM	117	OD1	ASN	A	16	32.261	13.260	8.533	1.00	32.71	A	O
ATOM	118	ND2	ASN	A	16	32.672	12.268	6.567	1.00	28.57	A	N
ATOM	119	C	ASN	A	16	30.491	8.811	7.692	1.00	21.95	A	C
ATOM	120	O	ASN	A	16	31.152	8.065	8.404	1.00	22.21	A	O
ATOM	121	N	PHE	A	17	29.203	8.578	7.438	1.00	20.66	A	N
ATOM	122	CA	PHE	A	17	28.550	7.392	8.003	1.00	20.24	A	C
ATOM	123	CB	PHE	A	17	27.415	7.815	8.938	1.00	21.09	A	C
ATOM	124	CG	PHE	A	17	27.890	8.591	10.134	1.00	19.81	A	C
ATOM	125	CD1	PHE	A	17	28.110	7.953	11.348	1.00	24.93	A	C
ATOM	126	CE1	PHE	A	17	28.556	8.679	12.459	1.00	25.33	A	C
ATOM	127	CZ	PHE	A	17	28.779	10.016	12.344	1.00	23.90	A	C
ATOM	128	CE2	PHE	A	17	28.564	10.651	11.155	1.00	22.65	A	C
ATOM	129	CD2	PHE	A	17	28.111	9.936	10.052	1.00	20.02	A	C
ATOM	130	C	PHE	A	17	28.061	6.385	6.977	1.00	19.13	A	C
ATOM	131	O	PHE	A	17	27.607	5.336	7.337	1.00	20.18	A	O
ATOM	132	N	GLY	A	18	28.205	6.685	5.692	1.00	17.84	A	N
ATOM	133	CA	GLY	A	18	27.740	5.790	4.640	1.00	17.25	A	C
ATOM	134	C	GLY	A	18	26.220	5.654	4.496	1.00	16.27	A	C
ATOM	135	O	GLY	A	18	25.755	4.667	3.948	1.00	14.47	A	O
ATOM	136	N	LEU	A	19	25.453	6.651	4.955	1.00	15.24	A	N
ATOM	137	CA	LEU	A	19	23.980	6.550	5.007	1.00	14.35	A	C
ATOM	138	CB	LEU	A	19	23.456	7.222	6.270	1.00	14.71	A	C
ATOM	139	CG	LEU	A	19	24.013	6.680	7.569	1.00	15.58	A	C
ATOM	140	CD1	LEU	A	19	23.691	7.633	8.721	1.00	16.09	A	C
ATOM	141	CD2	LEU	A	19	23.417	5.294	7.793	1.00	15.86	A	C
ATOM	142	C	LEU	A	19	23.305	7.203	3.820	1.00	13.82	A	C

ATOM	143	O	LEU	A	19	23.183	8.427	3.775	1.00	13.96	A	O
ATOM	144	N	TYR	A	20	22.874	6.400	2.854	1.00	13.81	A	N
ATOM	145	CA	TYR	A	20	22.156	6.917	1.714	1.00	14.22	A	C
ATOM	146	CB	TYR	A	20	22.841	6.499	0.386	1.00	14.36	A	C
ATOM	147	CG	TYR	A	20	24.254	7.034	0.241	1.00	14.09	A	C
ATOM	148	CD1	TYR	A	20	25.351	6.353	0.792	1.00	16.48	A	C
ATOM	149	CE1	TYR	A	20	26.661	6.858	0.663	1.00	16.91	A	C
ATOM	150	CZ	TYR	A	20	26.859	8.041	-0.034	1.00	18.57	A	C
ATOM	151	OH	TYR	A	20	28.126	8.567	-0.171	1.00	21.21	A	O
ATOM	152	CE2	TYR	A	20	25.788	8.735	-0.575	1.00	17.45	A	C
ATOM	153	CD2	TYR	A	20	24.495	8.217	-0.461	1.00	16.03	A	C
ATOM	154	C	TYR	A	20	20.715	6.433	1.702	1.00	14.55	A	C
ATOM	155	O	TYR	A	20	19.994	6.688	0.723	1.00	14.48	A	O
ATOM	156	N	GLY	A	21	20.297	5.710	2.746	1.00	14.18	A	N
ATOM	157	CA	GLY	A	21	18.947	5.172	2.802	1.00	14.23	A	C
ATOM	158	C	GLY	A	21	18.749	3.775	2.207	1.00	14.56	A	C
ATOM	159	O	GLY	A	21	17.611	3.315	2.054	1.00	13.53	A	O
ATOM	160	N	GLN	A	22	19.838	3.084	1.883	1.00	14.57	A	N
ATOM	161	CA	GLN	A	22	19.722	1.726	1.334	1.00	14.82	A	C
ATOM	162	CB	GLN	A	22	21.095	1.130	0.978	1.00	15.45	A	C
ATOM	163	CG	GLN	A	22	21.054	-0.151	0.150	1.00	17.91	A	C
ATOM	164	CD	GLN	A	22	20.669	-1.376	0.976	1.00	21.79	A	C
ATOM	165	OE1	GLN	A	22	20.892	-1.414	2.185	1.00	22.42	A	O
ATOM	166	NE2	GLN	A	22	20.091	-2.379	0.317	1.00	23.11	A	N
ATOM	167	C	GLN	A	22	19.011	0.831	2.331	1.00	14.04	A	C
ATOM	168	O	GLN	A	22	19.341	0.824	3.516	1.00	14.39	A	O
ATOM	169	N	GLY	A	23	18.019	0.110	1.836	1.00	14.26	A	N
ATOM	170	CA	GLY	A	23	17.236	-0.859	2.628	1.00	14.81	A	C
ATOM	171	C	GLY	A	23	15.957	-0.245	3.176	1.00	14.12	A	C
ATOM	172	O	GLY	A	23	15.086	-0.948	3.718	1.00	14.17	A	O
ATOM	173	N	GLN	A	24	15.836	1.077	3.057	1.00	13.54	A	N
ATOM	174	CA	GLN	A	24	14.620	1.773	3.500	1.00	13.27	A	C
ATOM	175	CB	GLN	A	24	14.963	3.090	4.182	1.00	12.64	A	C
ATOM	176	CG	GLN	A	24	15.806	2.945	5.450	1.00	13.46	A	C
ATOM	177	CD	GLN	A	24	15.150	2.100	6.505	1.00	15.72	A	C
ATOM	178	OE1	GLN	A	24	14.015	2.387	6.921	1.00	14.73	A	O
ATOM	179	NE2	GLN	A	24	15.839	1.026	6.927	1.00	13.89	A	N
ATOM	180	C	GLN	A	24	13.619	2.022	2.352	1.00	13.19	A	C
ATOM	181	O	GLN	A	24	14.005	2.126	1.184	1.00	13.48	A	O
ATOM	182	N	ILE	A	25	12.324	2.066	2.692	1.00	13.28	A	N
ATOM	183	CA	ILE	A	25	11.280	2.319	1.720	1.00	13.25	A	C
ATOM	184	CB	ILE	A	25	10.404	1.077	1.507	1.00	13.64	A	C
ATOM	185	CG1	ILE	A	25	11.267	-0.108	1.030	1.00	15.44	A	C
ATOM	186	CD1	ILE	A	25	10.508	-1.518	0.962	1.00	14.73	A	C
ATOM	187	CG2	ILE	A	25	9.303	1.387	0.503	1.00	13.37	A	C
ATOM	188	C	ILE	A	25	10.447	3.491	2.209	1.00	13.24	A	C
ATOM	189	O	ILE	A	25	9.884	3.430	3.285	1.00	12.93	A	O
ATOM	190	N	VAL	A	26	10.438	4.573	1.432	1.00	12.43	A	N
ATOM	191	CA	VAL	A	26	9.656	5.754	1.737	1.00	12.49	A	C
ATOM	192	CB	VAL	A	26	10.480	7.034	1.585	1.00	12.90	A	C
ATOM	193	CG1	VAL	A	26	9.671	8.231	2.059	1.00	11.57	A	C
ATOM	194	CG2	VAL	A	26	11.796	6.928	2.395	1.00	15.53	A	C
ATOM	195	C	VAL	A	26	8.465	5.823	0.804	1.00	12.34	A	C
ATOM	196	O	VAL	A	26	8.601	5.646	-0.418	1.00	11.99	A	O
ATOM	197	N	ALA	A	27	7.297	6.044	1.387	1.00	12.40	A	N
ATOM	198	CA	ALA	A	27	6.080	6.289	0.624	1.00	12.49	A	C
ATOM	199	CB	ALA	A	27	4.846	5.650	1.284	1.00	11.39	A	C
ATOM	200	C	ALA	A	27	5.892	7.790	0.546	1.00	12.17	A	C

ATOM	201	O	ALA	A	27	6.077	8.501	1.526	1.00	11.39	A	O
ATOM	202	N	VAL	A	28	5.540	8.243	-0.643	1.00	11.79	A	N
ATOM	203	CA	VAL	A	28	5.168	9.612	-0.910	1.00	11.63	A	C
ATOM	204	CB	VAL	A	28	6.054	10.176	-2.003	1.00	11.56	A	C
ATOM	205	CG1	VAL	A	28	5.629	11.625	-2.440	1.00	12.77	A	C
ATOM	206	CG2	VAL	A	28	7.514	10.079	-1.594	1.00	11.95	A	C
ATOM	207	C	VAL	A	28	3.729	9.580	-1.458	1.00	11.23	A	C
ATOM	208	O	VAL	A	28	3.470	8.936	-2.459	1.00	10.72	A	O
ATOM	209	N	ALA	A	29	2.817	10.294	-0.831	1.00	10.64	A	N
ATOM	210	CA	ALA	A	29	1.468	10.435	-1.365	1.00	11.32	A	C
ATOM	211	CB	ALA	A	29	0.441	10.151	-0.298	1.00	11.33	A	C
ATOM	212	C	ALA	A	29	1.326	11.842	-1.909	1.00	11.35	A	C
ATOM	213	O	ALA	A	29	1.404	12.826	-1.161	1.00	11.19	A	O
ATOM	214	N	ASP	A	30	1.186	11.937	-3.229	1.00	11.71	A	N
ATOM	215	CA	ASP	A	30	1.266	13.221	-3.917	1.00	11.52	A	C
ATOM	216	CB	ASP	A	30	2.718	13.715	-3.958	1.00	11.37	A	C
ATOM	217	CG	ASP	A	30	2.802	15.221	-3.852	1.00	12.40	A	C
ATOM	218	OD1	ASP	A	30	3.385	15.726	-2.871	1.00	12.15	A	O
ATOM	219	OD2	ASP	A	30	2.226	15.973	-4.682	1.00	14.39	A	O
ATOM	220	C	ASP	A	30	0.665	13.113	-5.327	1.00	12.41	A	C
ATOM	221	O	ASP	A	30	0.068	12.086	-5.671	1.00	12.89	A	O
ATOM	222	N	THR	A	31	0.811	14.162	-6.151	1.00	12.52	A	N
ATOM	223	CA	THR	A	31	-0.004	14.263	-7.353	1.00	11.62	A	C
ATOM	224	CB	THR	A	31	0.302	15.554	-8.182	1.00	11.72	A	C
ATOM	225	OG1	THR	A	31	1.709	15.702	-8.423	1.00	11.44	A	O
ATOM	226	CG2	THR	A	31	-0.099	16.789	-7.424	1.00	11.85	A	C
ATOM	227	C	THR	A	31	0.126	13.041	-8.225	1.00	12.59	A	C
ATOM	228	O	THR	A	31	-0.868	12.341	-8.494	1.00	12.63	A	O
ATOM	229	N	GLY	A	32	1.360	12.810	-8.665	1.00	12.03	A	N
ATOM	230	CA	GLY	A	32	1.694	11.788	-9.617	1.00	12.81	A	C
ATOM	231	C	GLY	A	32	3.202	11.763	-9.729	1.00	13.22	A	C
ATOM	232	O	GLY	A	32	3.885	12.607	-9.135	1.00	12.83	A	O
ATOM	233	N	LEU	A	33	3.711	10.813	-10.501	1.00	13.41	A	N
ATOM	234	CA	LEU	A	33	5.139	10.622	-10.678	1.00	13.86	A	C
ATOM	235	CB	LEU	A	33	5.625	9.397	-9.899	1.00	13.74	A	C
ATOM	236	CG	LEU	A	33	7.148	9.234	-9.900	1.00	14.12	A	C
ATOM	237	CD1	LEU	A	33	7.768	10.273	-8.964	1.00	13.99	A	C
ATOM	238	CD2	LEU	A	33	7.497	7.818	-9.437	1.00	15.42	A	C
ATOM	239	C	LEU	A	33	5.517	10.505	-12.151	1.00	13.89	A	C
ATOM	240	O	LEU	A	33	5.374	9.444	-12.765	1.00	14.14	A	O
ATOM	241	N	ASP	A	34	6.009	11.612	-12.696	1.00	14.55	A	N
ATOM	242	CA	ASP	A	34	6.455	11.701	-14.087	1.00	14.62	A	C
ATOM	243	CB	ASP	A	34	7.899	11.201	-14.224	1.00	14.72	A	C
ATOM	244	CG	ASP	A	34	8.516	11.532	-15.598	1.00	15.30	A	C
ATOM	245	OD1	ASP	A	34	9.260	10.694	-16.148	1.00	14.31	A	O
ATOM	246	OD2	ASP	A	34	8.268	12.602	-16.207	1.00	17.33	A	O
ATOM	247	C	ASP	A	34	5.470	11.016	-15.060	1.00	14.94	A	C
ATOM	248	O	ASP	A	34	4.297	11.415	-15.124	1.00	15.39	A	O
ATOM	249	N	THR	A	35	5.927	10.013	-15.816	1.00	16.25	A	N
ATOM	250	CA	THR	A	35	5.083	9.340	-16.813	1.00	16.50	A	C
ATOM	251	CB	THR	A	35	5.912	8.471	-17.786	1.00	17.03	A	C
ATOM	252	OG1	THR	A	35	6.700	7.514	-17.051	1.00	17.34	A	O
ATOM	253	CG2	THR	A	35	6.922	9.300	-18.593	1.00	17.53	A	C
ATOM	254	C	THR	A	35	4.005	8.437	-16.229	1.00	17.26	A	C
ATOM	255	O	THR	A	35	3.111	7.992	-16.946	1.00	15.49	A	O
ATOM	256	N	GLY	A	36	4.104	8.104	-14.948	1.00	16.59	A	N
ATOM	257	CA	GLY	A	36	3.094	7.259	-14.360	1.00	16.76	A	C
ATOM	258	C	GLY	A	36	3.308	5.802	-14.660	1.00	17.58	A	C



ATOM	259	O	GLY	A	36	2.432	4.984	-14.383	1.00	17.55	A	O
ATOM	260	N	ARG	A	37	4.473	5.465	-15.200	1.00	18.31	A	N
ATOM	261	CA	ARG	A	37	4.748	4.091	-15.575	1.00	19.42	A	C
ATOM	262	CB	ARG	A	37	4.763	3.940	-17.088	1.00	20.37	A	C
ATOM	263	CG	ARG	A	37	3.436	4.298	-17.742	1.00	23.71	A	C
ATOM	264	CD	ARG	A	37	3.283	3.740	-19.140	1.00	31.29	A	C
ATOM	265	NE	ARG	A	37	4.324	4.233	-20.024	1.00	34.29	A	N
ATOM	266	CZ	ARG	A	37	4.322	5.434	-20.575	1.00	38.63	A	C
ATOM	267	NH1	ARG	A	37	5.331	5.792	-21.361	1.00	39.90	A	N
ATOM	268	NH2	ARG	A	37	3.305	6.273	-20.362	1.00	40.23	A	N
ATOM	269	C	ARG	A	37	6.072	3.661	-14.998	1.00	19.41	A	C
ATOM	270	O	ARG	A	37	7.065	4.354	-15.150	1.00	18.12	A	O
ATOM	271	N	ASN	A	38	6.067	2.506	-14.334	1.00	19.47	A	N
ATOM	272	CA	ASN	A	38	7.254	1.998	-13.703	1.00	20.37	A	C
ATOM	273	CB	ASN	A	38	6.917	1.215	-12.431	1.00	20.71	A	C
ATOM	274	CG	ASN	A	38	8.161	0.841	-11.658	1.00	21.12	A	C
ATOM	275	OD1	ASN	A	38	9.248	1.337	-11.968	1.00	18.41	A	O
ATOM	276	ND2	ASN	A	38	8.023	-0.072	-10.684	1.00	20.60	A	N
ATOM	277	C	ASN	A	38	7.984	1.134	-14.700	1.00	21.21	A	C
ATOM	278	O	ASN	A	38	7.918	-0.099	-14.638	1.00	21.03	A	O
ATOM	279	N	ASP	A	39	8.659	1.806	-15.625	1.00	21.69	A	N
ATOM	280	CA	ASP	A	39	9.363	1.158	-16.718	1.00	23.22	A	C
ATOM	281	CB	ASP	A	39	8.405	0.839	-17.882	1.00	23.19	A	C
ATOM	282	CG	ASP	A	39	7.806	2.082	-18.526	1.00	24.66	A	C
ATOM	283	OD1	ASP	A	39	6.796	1.945	-19.248	1.00	26.50	A	O
ATOM	284	OD2	ASP	A	39	8.246	3.239	-18.372	1.00	27.03	A	O
ATOM	285	C	ASP	A	39	10.480	2.075	-17.156	1.00	24.00	A	C
ATOM	286	O	ASP	A	39	10.843	3.004	-16.434	1.00	23.68	A	O
ATOM	287	N	SER	A	40	11.003	1.832	-18.355	1.00	24.67	A	N
ATOM	288	CA	SER	A	40	12.166	2.539	-18.847	1.00	24.80	A	C
ATOM	289	CB	SER	A	40	12.777	1.766	-20.041	1.00	25.30	A	C
ATOM	290	OG	SER	A	40	11.925	1.881	-21.163	1.00	25.60	A	O
ATOM	291	C	SER	A	40	11.815	3.984	-19.228	1.00	23.51	A	C
ATOM	292	O	SER	A	40	12.687	4.805	-19.375	1.00	24.41	A	O
ATOM	293	N	SER	A	41	10.532	4.308	-19.317	1.00	23.14	A	N
ATOM	294	CA	SER	A	41	10.097	5.670	-19.621	1.00	21.75	A	C
ATOM	295	CB	SER	A	41	8.620	5.679	-20.037	1.00	22.84	A	C
ATOM	296	OG	SER	A	41	7.725	5.739	-18.919	1.00	21.43	A	O
ATOM	297	C	SER	A	41	10.262	6.639	-18.427	1.00	21.13	A	C
ATOM	298	O	SER	A	41	10.299	7.863	-18.603	1.00	19.88	A	O
ATOM	299	N	MET	A	42	10.359	6.079	-17.223	1.00	19.68	A	N
ATOM	300	CA	MET	A	42	10.381	6.882	-15.996	1.00	18.70	A	C
ATOM	301	CB	MET	A	42	10.295	5.949	-14.782	1.00	18.20	A	C
ATOM	302	CG	MET	A	42	10.451	6.626	-13.423	1.00	17.87	A	C
ATOM	303	SD	MET	A	42	9.190	7.804	-13.030	1.00	16.31	A	S
ATOM	304	CE	MET	A	42	7.658	6.844	-13.134	1.00	15.38	A	C
ATOM	305	C	MET	A	42	11.607	7.779	-15.897	1.00	17.89	A	C
ATOM	306	O	MET	A	42	12.728	7.390	-16.223	1.00	17.28	A	O
ATOM	307	N	HIS	A	43	11.381	8.998	-15.421	1.00	17.69	A	N
ATOM	308	CA	HIS	A	43	12.479	9.903	-15.081	1.00	17.38	A	C
ATOM	309	CB	HIS	A	43	11.942	11.020	-14.196	1.00	17.29	A	C
ATOM	310	CG	HIS	A	43	12.896	12.155	-13.981	1.00	16.73	A	C
ATOM	311	ND1	HIS	A	43	12.576	13.456	-14.321	1.00	16.98	A	N
ATOM	312	CE1	HIS	A	43	13.566	14.257	-13.971	1.00	13.61	A	C
ATOM	313	NE2	HIS	A	43	14.521	13.523	-13.426	1.00	17.49	A	N
ATOM	314	CD2	HIS	A	43	14.113	12.207	-13.397	1.00	13.70	A	C
ATOM	315	C	HIS	A	43	13.647	9.209	-14.381	1.00	16.64	A	C
ATOM	316	O	HIS	A	43	13.453	8.389	-13.479	1.00	15.82	A	O



ATOM	317	N	GLU	A	44	14.858	9.559	-14.818	1.00	16.35	A	N
ATOM	318	CA	GLU	A	44	16.112	8.985	-14.358	1.00	16.74	A	C
ATOM	319	CB	GLU	A	44	17.293	9.763	-14.988	1.00	17.71	A	C
ATOM	320	CG	GLU	A	44	17.268	11.270	-14.753	1.00	18.20	A	C
ATOM	321	CD	GLU	A	44	18.445	12.004	-15.418	1.00	22.20	A	C
ATOM	322	OE1	GLU	A	44	18.997	11.455	-16.397	1.00	20.94	A	O
ATOM	323	OE2	GLU	A	44	18.843	13.110	-14.933	1.00	20.93	A	O
ATOM	324	C	GLU	A	44	16.280	8.982	-12.823	1.00	17.11	A	C
ATOM	325	O	GLU	A	44	16.944	8.104	-12.259	1.00	17.08	A	O
ATOM	326	N	ALA	A	45	15.665	9.954	-12.152	1.00	16.39	A	N
ATOM	327	CA	ALA	A	45	15.774	10.061	-10.696	1.00	16.01	A	C
ATOM	328	CB	ALA	A	45	15.122	11.354	-10.198	1.00	15.44	A	C
ATOM	329	C	ALA	A	45	15.155	8.864	-9.971	1.00	16.39	A	C
ATOM	330	O	ALA	A	45	15.538	8.564	-8.857	1.00	14.42	A	O
ATOM	331	N	PHE	A	46	14.184	8.218	-10.595	1.00	16.01	A	N
ATOM	332	CA	PHE	A	46	13.411	7.139	-9.971	1.00	16.28	A	C
ATOM	333	CB	PHE	A	46	11.958	7.562	-9.882	1.00	16.14	A	C
ATOM	334	CG	PHE	A	46	11.780	8.959	-9.396	1.00	14.90	A	C
ATOM	335	CD1	PHE	A	46	12.036	9.275	-8.078	1.00	14.17	A	C
ATOM	336	CE1	PHE	A	46	11.897	10.586	-7.628	1.00	13.19	A	C
ATOM	337	CZ	PHE	A	46	11.525	11.592	-8.504	1.00	14.92	A	C
ATOM	338	CE2	PHE	A	46	11.291	11.299	-9.809	1.00	16.01	A	C
ATOM	339	CD2	PHE	A	46	11.416	9.971	-10.261	1.00	15.93	A	C
ATOM	340	C	PHE	A	46	13.466	5.791	-10.697	1.00	17.23	A	C
ATOM	341	O	PHE	A	46	13.017	4.764	-10.172	1.00	16.06	A	O
ATOM	342	N	ARG	A	47	13.986	5.781	-11.917	1.00	18.87	A	N
ATOM	343	CA	ARG	A	47	13.963	4.566	-12.723	1.00	20.32	A	C
ATOM	344	CB	ARG	A	47	14.659	4.833	-14.062	1.00	21.00	A	C
ATOM	345	CG	ARG	A	47	14.309	3.871	-15.173	1.00	24.13	A	C
ATOM	346	CD	ARG	A	47	14.468	4.517	-16.570	1.00	28.53	A	C
ATOM	347	NE	ARG	A	47	15.803	5.031	-16.813	1.00	32.22	A	N
ATOM	348	CZ	ARG	A	47	16.105	6.229	-17.359	1.00	34.45	A	C
ATOM	349	NH1	ARG	A	47	15.171	7.109	-17.703	1.00	33.97	A	N
ATOM	350	NH2	ARG	A	47	17.384	6.558	-17.527	1.00	33.82	A	N
ATOM	351	C	ARG	A	47	14.674	3.437	-12.000	1.00	20.49	A	C
ATOM	352	O	ARG	A	47	15.784	3.619	-11.523	1.00	21.38	A	O
ATOM	353	N	GLY	A	48	14.032	2.280	-11.898	1.00	21.45	A	N
ATOM	354	CA	GLY	A	48	14.642	1.105	-11.274	1.00	21.59	A	C
ATOM	355	C	GLY	A	48	14.583	1.091	-9.741	1.00	21.98	A	C
ATOM	356	O	GLY	A	48	15.072	0.145	-9.102	1.00	21.74	A	O
ATOM	357	N	LYS	A	49	13.984	2.117	-9.136	1.00	21.05	A	N
ATOM	358	CA	LYS	A	49	13.950	2.197	-7.662	1.00	20.90	A	C
ATOM	359	CB	LYS	A	49	14.915	3.305	-7.180	1.00	22.03	A	C
ATOM	360	CG	LYS	A	49	14.366	4.713	-7.161	1.00	24.83	A	C
ATOM	361	CD	LYS	A	49	15.447	5.815	-6.761	1.00	27.45	A	C
ATOM	362	CE	LYS	A	49	15.957	5.680	-5.358	1.00	27.82	A	C
ATOM	363	NZ	LYS	A	49	17.024	4.667	-5.220	1.00	28.25	A	N
ATOM	364	C	LYS	A	49	12.523	2.329	-7.077	1.00	19.90	A	C
ATOM	365	O	LYS	A	49	12.339	2.667	-5.890	1.00	19.91	A	O
ATOM	366	N	ILE	A	50	11.523	1.999	-7.900	1.00	18.63	A	N
ATOM	367	CA	ILE	A	50	10.121	2.078	-7.533	1.00	17.48	A	C
ATOM	368	CB	ILE	A	50	9.284	2.650	-8.695	1.00	17.67	A	C
ATOM	369	CG1	ILE	A	50	9.738	4.076	-9.050	1.00	17.24	A	C
ATOM	370	CD1	ILE	A	50	9.083	4.630	-10.302	1.00	17.34	A	C
ATOM	371	CG2	ILE	A	50	7.807	2.723	-8.319	1.00	17.29	A	C
ATOM	372	C	ILE	A	50	9.562	0.730	-7.090	1.00	17.96	A	C
ATOM	373	O	ILE	A	50	9.339	-0.161	-7.909	1.00	18.69	A	O
ATOM	374	N	THR	A	51	9.355	0.583	-5.784	1.00	17.09	A	N

ATOM	375	CA	THR	A	51	8.731	-0.601	-5.218	1.00	17.60	A	C
ATOM	376	CB	THR	A	51	8.700	-0.423	-3.690	1.00	18.38	A	C
ATOM	377	OG1	THR	A	51	10.033	-0.380	-3.205	1.00	17.39	A	O
ATOM	378	CG2	THR	A	51	8.054	-1.617	-3.014	1.00	17.34	A	C
ATOM	379	C	THR	A	51	7.301	-0.746	-5.646	1.00	17.50	A	C
ATOM	380	O	THR	A	51	6.827	-1.834	-5.903	1.00	18.10	A	O
ATOM	381	N	ALA	A	52	6.578	0.369	-5.670	1.00	16.93	A	N
ATOM	382	CA	ALA	A	52	5.179	0.338	-6.052	1.00	17.34	A	C
ATOM	383	CB	ALA	A	52	4.314	-0.132	-4.884	1.00	17.41	A	C
ATOM	384	C	ALA	A	52	4.753	1.725	-6.501	1.00	17.46	A	C
ATOM	385	O	ALA	A	52	5.187	2.730	-5.928	1.00	16.50	A	O
ATOM	386	N	LEU	A	53	3.921	1.760	-7.539	1.00	17.19	A	N
ATOM	387	CA	LEU	A	53	3.369	2.987	-8.081	1.00	16.89	A	C
ATOM	388	CB	LEU	A	53	4.004	3.309	-9.430	1.00	16.66	A	C
ATOM	389	CG	LEU	A	53	3.490	4.525	-10.224	1.00	16.83	A	C
ATOM	390	CD1	LEU	A	53	3.523	5.796	-9.401	1.00	15.83	A	C
ATOM	391	CD2	LEU	A	53	4.303	4.720	-11.476	1.00	17.71	A	C
ATOM	392	C	LEU	A	53	1.868	2.779	-8.212	1.00	17.28	A	C
ATOM	393	O	LEU	A	53	1.421	2.057	-9.097	1.00	17.43	A	O
ATOM	394	N	TYR	A	54	1.101	3.393	-7.303	1.00	17.28	A	N
ATOM	395	CA	TYR	A	54	-0.350	3.200	-7.230	1.00	16.87	A	C
ATOM	396	CB	TYR	A	54	-0.774	2.944	-5.789	1.00	16.88	A	C
ATOM	397	CG	TYR	A	54	-0.268	1.679	-5.144	1.00	15.63	A	C
ATOM	398	CD1	TYR	A	54	-0.411	0.448	-5.770	1.00	15.86	A	C
ATOM	399	CE1	TYR	A	54	0.037	-0.698	-5.192	1.00	15.12	A	C
ATOM	400	CZ	TYR	A	54	0.666	-0.647	-3.946	1.00	15.32	A	C
ATOM	401	OH	TYR	A	54	1.093	-1.815	-3.374	1.00	14.97	A	O
ATOM	402	CE2	TYR	A	54	0.856	0.558	-3.312	1.00	15.70	A	C
ATOM	403	CD2	TYR	A	54	0.384	1.718	-3.908	1.00	15.59	A	C
ATOM	404	C	TYR	A	54	-1.098	4.411	-7.712	1.00	17.11	A	C
ATOM	405	O	TYR	A	54	-0.733	5.546	-7.387	1.00	16.78	A	O
ATOM	406	N	ALA	A	55	-2.161	4.184	-8.483	1.00	17.01	A	N
ATOM	407	CA	ALA	A	55	-3.032	5.260	-8.926	1.00	17.49	A	C
ATOM	408	CB	ALA	A	55	-3.355	5.094	-10.437	1.00	17.43	A	C
ATOM	409	C	ALA	A	55	-4.323	5.272	-8.100	1.00	18.26	A	C
ATOM	410	O	ALA	A	55	-5.174	4.400	-8.269	1.00	19.60	A	O
ATOM	411	N	LEU	A	56	-4.481	6.267	-7.230	1.00	17.69	A	N
ATOM	412	CA	LEU	A	56	-5.641	6.353	-6.368	1.00	17.32	A	C
ATOM	413	CB	LEU	A	56	-5.224	6.779	-4.965	1.00	16.99	A	C
ATOM	414	CG	LEU	A	56	-4.452	5.752	-4.129	1.00	17.97	A	C
ATOM	415	CD1	LEU	A	56	-3.120	5.532	-4.719	1.00	20.33	A	C
ATOM	416	CD2	LEU	A	56	-4.329	6.225	-2.662	1.00	19.18	A	C
ATOM	417	C	LEU	A	56	-6.662	7.360	-6.867	1.00	17.28	A	C
ATOM	418	O	LEU	A	56	-7.839	7.192	-6.653	1.00	17.95	A	O
ATOM	419	N	GLY	A	57	-6.204	8.430	-7.485	1.00	17.26	A	N
ATOM	420	CA	GLY	A	57	-7.068	9.541	-7.802	1.00	17.53	A	C
ATOM	421	C	GLY	A	57	-7.662	9.430	-9.199	1.00	17.74	A	C
ATOM	422	O	GLY	A	57	-8.758	9.905	-9.446	1.00	17.69	A	O
ATOM	423	N	ARG	A	58	-6.921	8.825	-10.109	1.00	18.54	A	N
ATOM	424	CA	ARG	A	58	-7.361	8.659	-11.502	1.00	19.44	A	C
ATOM	425	CB	ARG	A	58	-6.572	9.555	-12.466	1.00	18.56	A	C
ATOM	426	CG	ARG	A	58	-6.873	11.036	-12.371	1.00	18.16	A	C
ATOM	427	CD	ARG	A	58	-5.685	11.912	-12.787	1.00	17.99	A	C
ATOM	428	NE	ARG	A	58	-4.505	11.593	-11.990	1.00	17.16	A	N
ATOM	429	CZ	ARG	A	58	-3.248	11.716	-12.392	1.00	18.78	A	C
ATOM	430	NH1	ARG	A	58	-2.967	12.194	-13.591	1.00	18.96	A	N
ATOM	431	NH2	ARG	A	58	-2.253	11.339	-11.584	1.00	17.60	A	N
ATOM	432	C	ARG	A	58	-7.123	7.240	-11.909	1.00	19.97	A	C

ATOM	433	O	ARG	A	58	-6.007	6.754	-11.878	1.00	20.06	A	O
ATOM	434	N	THR	A	59	-8.183	6.575	-12.324	1.00	22.06	A	N
ATOM	435	CA	THR	A	59	-8.091	5.180	-12.688	1.00	22.88	A	C
ATOM	436	CB	THR	A	59	-9.479	4.693	-13.142	1.00	24.04	A	C
ATOM	437	OG1	THR	A	59	-10.330	4.643	-11.984	1.00	25.24	A	O
ATOM	438	CG2	THR	A	59	-9.406	3.250	-13.657	1.00	25.24	A	C
ATOM	439	C	THR	A	59	-7.009	4.919	-13.733	1.00	22.06	A	C
ATOM	440	O	THR	A	59	-7.020	5.482	-14.835	1.00	22.93	A	O
ATOM	441	N	ASN	A	60	-6.074	4.068	-13.332	1.00	21.27	A	N
ATOM	442	CA	ASN	A	60	-4.939	3.618	-14.124	1.00	21.57	A	C
ATOM	443	CB	ASN	A	60	-5.400	2.788	-15.326	1.00	22.51	A	C
ATOM	444	CG	ASN	A	60	-5.861	1.401	-14.927	1.00	24.76	A	C
ATOM	445	OD1	ASN	A	60	-5.546	0.908	-13.835	1.00	27.82	A	O
ATOM	446	ND2	ASN	A	60	-6.624	0.773	-15.801	1.00	25.97	A	N
ATOM	447	C	ASN	A	60	-4.038	4.744	-14.614	1.00	20.35	A	C
ATOM	448	O	ASN	A	60	-3.369	4.589	-15.629	1.00	20.71	A	O
ATOM	449	N	ASN	A	61	-4.023	5.852	-13.897	1.00	18.43	A	N
ATOM	450	CA	ASN	A	61	-3.217	6.996	-14.300	1.00	18.53	A	C
ATOM	451	CB	ASN	A	61	-4.095	8.062	-14.972	1.00	17.54	A	C
ATOM	452	CG	ASN	A	61	-3.278	9.194	-15.580	1.00	19.62	A	C
ATOM	453	OD1	ASN	A	61	-3.832	10.171	-16.141	1.00	22.44	A	O
ATOM	454	ND2	ASN	A	61	-1.968	9.081	-15.481	1.00	15.52	A	N
ATOM	455	C	ASN	A	61	-2.520	7.586	-13.088	1.00	16.75	A	C
ATOM	456	O	ASN	A	61	-3.159	8.213	-12.260	1.00	16.00	A	O
ATOM	457	N	ALA	A	62	-1.219	7.357	-12.988	1.00	16.29	A	N
ATOM	458	CA	ALA	A	62	-0.418	7.910	-11.902	1.00	16.34	A	C
ATOM	459	CB	ALA	A	62	0.310	6.804	-11.183	1.00	16.55	A	C
ATOM	460	C	ALA	A	62	0.584	8.948	-12.405	1.00	16.52	A	C
ATOM	461	O	ALA	A	62	1.583	9.221	-11.728	1.00	15.61	A	O
ATOM	462	N	ASN	A	63	0.344	9.515	-13.593	1.00	15.91	A	N
ATOM	463	CA	ASN	A	63	1.276	10.465	-14.157	1.00	15.75	A	C
ATOM	464	CB	ASN	A	63	1.251	10.471	-15.720	1.00	15.36	A	C
ATOM	465	CG	ASN	A	63	0.043	11.165	-16.307	1.00	16.00	A	C
ATOM	466	OD1	ASN	A	63	-0.617	11.982	-15.643	1.00	14.50	A	O
ATOM	467	ND2	ASN	A	63	-0.274	10.833	-17.584	1.00	15.36	A	N
ATOM	468	C	ASN	A	63	1.115	11.858	-13.518	1.00	15.21	A	C
ATOM	469	O	ASN	A	63	0.168	12.108	-12.762	1.00	15.63	A	O
ATOM	470	N	ASP	A	64	2.047	12.753	-13.828	1.00	15.12	A	N
ATOM	471	CA	ASP	A	64	2.192	14.015	-13.102	1.00	15.29	A	C
ATOM	472	CB	ASP	A	64	3.450	13.990	-12.233	1.00	14.59	A	C
ATOM	473	CG	ASP	A	64	3.532	15.161	-11.300	1.00	15.31	A	C
ATOM	474	OD1	ASP	A	64	2.476	15.813	-11.058	1.00	14.15	A	O
ATOM	475	OD2	ASP	A	64	4.626	15.516	-10.776	1.00	14.37	A	O
ATOM	476	C	ASP	A	64	2.236	15.206	-14.061	1.00	15.53	A	C
ATOM	477	O	ASP	A	64	3.315	15.713	-14.423	1.00	16.54	A	O
ATOM	478	N	PRO	A	65	1.065	15.644	-14.476	1.00	16.18	A	N
ATOM	479	CA	PRO	A	65	0.950	16.813	-15.343	1.00	17.33	A	C
ATOM	480	CB	PRO	A	65	-0.509	16.776	-15.807	1.00	17.19	A	C
ATOM	481	CG	PRO	A	65	-1.225	15.953	-14.808	1.00	17.73	A	C
ATOM	482	CD	PRO	A	65	-0.249	15.043	-14.172	1.00	17.21	A	C
ATOM	483	C	PRO	A	65	1.228	18.102	-14.607	1.00	17.72	A	C
ATOM	484	O	PRO	A	65	1.515	19.081	-15.250	1.00	17.98	A	O
ATOM	485	N	ASN	A	66	1.150	18.065	-13.279	1.00	18.27	A	N
ATOM	486	CA	ASN	A	66	1.314	19.217	-12.426	1.00	19.24	A	C
ATOM	487	CB	ASN	A	66	0.536	18.958	-11.111	1.00	20.48	A	C
ATOM	488	CG	ASN	A	66	0.790	19.993	-10.068	1.00	22.89	A	C
ATOM	489	OD1	ASN	A	66	1.942	20.281	-9.721	1.00	23.54	A	O
ATOM	490	ND2	ASN	A	66	-0.287	20.591	-9.566	1.00	25.20	A	N

ATOM	491	C	ASN	A	66	2.806	19.457	-12.153	1.00	18.71	A	C
ATOM	492	O	ASN	A	66	3.314	20.549	-12.353	1.00	18.84	A	O
ATOM	493	N	GLY	A	67	3.500	18.426	-11.698	1.00	17.55	A	N
ATOM	494	CA	GLY	A	67	4.917	18.503	-11.406	1.00	16.38	A	C
ATOM	495	C	GLY	A	67	5.234	18.455	-9.916	1.00	15.32	A	C
ATOM	496	O	GLY	A	67	6.383	18.167	-9.542	1.00	15.11	A	O
ATOM	497	N	HIS	A	68	4.230	18.722	-9.075	1.00	13.44	A	N
ATOM	498	CA	HIS	A	68	4.406	18.776	-7.608	1.00	12.51	A	C
ATOM	499	CB	BHIS	A	68	3.109	19.121	-6.891	0.50	12.22	A	C
ATOM	500	CB	AHIS	A	68	3.048	19.078	-6.930	0.50	12.48	A	C
ATOM	501	CG	BHIS	A	68	3.266	19.371	-5.417	0.50	10.61	A	C
ATOM	502	CG	AHIS	A	68	3.140	19.398	-5.464	0.50	10.86	A	C
ATOM	503	ND1	BHIS	A	68	2.741	18.522	-4.453	0.50	5.34	A	N
ATOM	504	ND1	AHIS	A	68	3.742	18.559	-4.548	0.50	7.56	A	N
ATOM	505	CE1	BHIS	A	68	3.009	19.016	-3.254	0.50	6.59	A	C
ATOM	506	CE1	AHIS	A	68	3.674	19.102	-3.341	0.50	2.00	A	C
ATOM	507	NE2	BHIS	A	68	3.678	20.158	-3.403	0.50	7.98	A	N
ATOM	508	NE2	AHIS	A	68	3.061	20.277	-3.442	0.50	6.21	A	N
ATOM	509	CD2	BHIS	A	68	3.845	20.405	-4.745	0.50	5.10	A	C
ATOM	510	CD2	AHIS	A	68	2.697	20.471	-4.756	0.50	8.79	A	C
ATOM	511	C	HIS	A	68	4.986	17.474	-7.064	1.00	12.70	A	C
ATOM	512	O	HIS	A	68	6.025	17.471	-6.401	1.00	12.91	A	O
ATOM	513	N	GLY	A	69	4.315	16.374	-7.317	1.00	13.22	A	N
ATOM	514	CA	GLY	A	69	4.709	15.094	-6.739	1.00	13.52	A	C
ATOM	515	C	GLY	A	69	6.039	14.574	-7.181	1.00	13.01	A	C
ATOM	516	O	GLY	A	69	6.751	13.894	-6.418	1.00	13.80	A	O
ATOM	517	N	THR	A	70	6.391	14.865	-8.432	1.00	13.25	A	N
ATOM	518	CA	THR	A	70	7.651	14.425	-8.970	1.00	12.89	A	C
ATOM	519	CB	THR	A	70	7.688	14.638	-10.507	1.00	13.93	A	C
ATOM	520	OG1	THR	A	70	6.592	13.940	-11.116	1.00	14.34	A	O
ATOM	521	CG2	THR	A	70	8.895	13.977	-11.110	1.00	13.50	A	C
ATOM	522	C	THR	A	70	8.769	15.192	-8.309	1.00	12.86	A	C
ATOM	523	O	THR	A	70	9.816	14.622	-8.013	1.00	13.63	A	O
ATOM	524	N	HIS	A	71	8.560	16.498	-8.093	1.00	12.19	A	N
ATOM	525	CA	HIS	A	71	9.580	17.341	-7.486	1.00	11.80	A	C
ATOM	526	CB	HIS	A	71	9.125	18.796	-7.555	1.00	11.41	A	C
ATOM	527	CG	BHIS	A	71	10.185	19.784	-7.212	0.50	11.89	A	C
ATOM	528	CG	AHIS	A	71	10.189	19.775	-7.181	0.50	9.73	A	C
ATOM	529	ND1	BHIS	A	71	10.926	19.709	-6.050	0.50	12.60	A	N
ATOM	530	ND1	AHIS	A	71	10.236	20.388	-5.942	0.50	5.89	A	N
ATOM	531	CE1	BHIS	A	71	11.791	20.706	-6.025	0.50	13.16	A	C
ATOM	532	CE1	AHIS	A	71	11.281	21.192	-5.898	0.50	7.95	A	C
ATOM	533	NE2	BHIS	A	71	11.618	21.438	-7.114	0.50	14.18	A	N
ATOM	534	NE2	AHIS	A	71	11.923	21.107	-7.054	0.50	10.14	A	N
ATOM	535	CD2	BHIS	A	71	10.617	20.883	-7.869	0.50	10.25	A	C
ATOM	536	CD2	AHIS	A	71	11.258	20.231	-7.874	0.50	6.22	A	C
ATOM	537	C	HIS	A	71	9.806	16.875	-6.018	1.00	12.35	A	C
ATOM	538	O	HIS	A	71	10.935	16.698	-5.538	1.00	12.45	A	O
ATOM	539	N	VAL	A	72	8.697	16.657	-5.331	1.00	12.33	A	N
ATOM	540	CA	VAL	A	72	8.704	16.204	-3.960	1.00	12.62	A	C
ATOM	541	CB	VAL	A	72	7.279	16.056	-3.469	1.00	12.75	A	C
ATOM	542	CG1	VAL	A	72	7.248	15.256	-2.202	1.00	12.50	A	C
ATOM	543	CG2	VAL	A	72	6.647	17.430	-3.262	1.00	12.97	A	C
ATOM	544	C	VAL	A	72	9.431	14.864	-3.799	1.00	13.01	A	C
ATOM	545	O	VAL	A	72	10.333	14.707	-2.947	1.00	12.02	A	O
ATOM	546	N	ALA	A	73	9.054	13.888	-4.615	1.00	12.23	A	N
ATOM	547	CA	ALA	A	73	9.664	12.572	-4.521	1.00	12.29	A	C
ATOM	548	CB	ALA	A	73	8.986	11.617	-5.440	1.00	12.32	A	C



ATOM	549	C	ALA	A	73	11.180	12.682	-4.850	1.00	11.78	A	C
ATOM	550	O	ALA	A	73	11.985	11.992	-4.280	1.00	11.60	A	O
ATOM	551	N	GLY	A	74	11.553	13.583	-5.742	1.00	12.04	A	N
ATOM	552	CA	GLY	A	74	12.961	13.760	-6.069	1.00	11.92	A	C
ATOM	553	C	GLY	A	74	13.768	14.190	-4.845	1.00	12.13	A	C
ATOM	554	O	GLY	A	74	14.936	13.816	-4.693	1.00	11.64	A	O
ATOM	555	N	SER	A	75	13.157	15.015	-3.994	1.00	12.08	A	N
ATOM	556	CA	SER	A	75	13.844	15.546	-2.827	1.00	12.08	A	C
ATOM	557	CB	SER	A	75	13.095	16.748	-2.267	1.00	11.53	A	C
ATOM	558	OG	SER	A	75	13.254	17.915	-3.077	1.00	13.29	A	O
ATOM	559	C	SER	A	75	14.033	14.477	-1.739	1.00	12.05	A	C
ATOM	560	O	SER	A	75	14.984	14.540	-0.927	1.00	12.73	A	O
ATOM	561	N	VAL	A	76	13.112	13.524	-1.676	1.00	11.61	A	N
ATOM	562	CA	VAL	A	76	13.272	12.407	-0.748	1.00	11.87	A	C
ATOM	563	CB	VAL	A	76	12.023	11.519	-0.691	1.00	12.06	A	C
ATOM	564	CG1	VAL	A	76	12.224	10.396	0.324	1.00	12.75	A	C
ATOM	565	CG2	VAL	A	76	10.799	12.319	-0.316	1.00	11.56	A	C
ATOM	566	C	VAL	A	76	14.415	11.501	-1.173	1.00	12.11	A	C
ATOM	567	O	VAL	A	76	15.280	11.158	-0.372	1.00	10.37	A	O
ATOM	568	N	LEU	A	77	14.410	11.085	-2.437	1.00	12.79	A	N
ATOM	569	CA	LEU	A	77	15.234	9.934	-2.809	1.00	12.61	A	C
ATOM	570	CB	LEU	A	77	14.532	8.627	-2.425	1.00	13.05	A	C
ATOM	571	CG	LEU	A	77	13.050	8.419	-2.774	1.00	11.85	A	C
ATOM	572	CD1	LEU	A	77	12.868	8.361	-4.281	1.00	12.80	A	C
ATOM	573	CD2	LEU	A	77	12.512	7.140	-2.114	1.00	14.07	A	C
ATOM	574	C	LEU	A	77	15.676	9.847	-4.267	1.00	13.21	A	C
ATOM	575	O	LEU	A	77	16.181	8.810	-4.656	1.00	13.59	A	O
ATOM	576	N	GLY	A	78	15.586	10.935	-5.022	1.00	13.72	A	N
ATOM	577	CA	GLY	A	78	16.045	10.945	-6.415	1.00	14.19	A	C
ATOM	578	C	GLY	A	78	17.486	10.505	-6.506	1.00	14.88	A	C
ATOM	579	O	GLY	A	78	18.322	10.998	-5.718	1.00	14.70	A	O
ATOM	580	N	ASN	A	79	17.800	9.587	-7.420	1.00	15.24	A	N
ATOM	581	CA	ASN	A	79	19.172	9.066	-7.520	1.00	16.71	A	C
ATOM	582	CB	ASN	A	79	19.204	7.542	-7.263	1.00	16.08	A	C
ATOM	583	CG	ASN	A	79	20.615	7.023	-6.904	1.00	16.70	A	C
ATOM	584	OD1	ASN	A	79	21.438	7.754	-6.372	1.00	15.21	A	O
ATOM	585	ND2	ASN	A	79	20.881	5.749	-7.181	1.00	15.92	A	N
ATOM	586	C	ASN	A	79	19.877	9.353	-8.852	1.00	18.12	A	C
ATOM	587	O	ASN	A	79	20.735	8.576	-9.267	1.00	18.96	A	O
ATOM	588	N	ALA	A	80	19.559	10.458	-9.513	1.00	18.68	A	N
ATOM	589	CA	ALA	A	80	20.316	10.838	-10.723	1.00	19.08	A	C
ATOM	590	CB	ALA	A	80	19.381	11.169	-11.876	1.00	19.15	A	C
ATOM	591	C	ALA	A	80	21.261	11.995	-10.376	1.00	18.85	A	C
ATOM	592	O	ALA	A	80	22.245	11.795	-9.663	1.00	18.76	A	O
ATOM	593	N	THR	A	81	20.973	13.194	-10.841	1.00	18.39	A	N
ATOM	594	CA	THR	A	81	21.647	14.370	-10.305	1.00	18.18	A	C
ATOM	595	CB	THR	A	81	22.229	15.222	-11.444	1.00	18.72	A	C
ATOM	596	OG1	THR	A	81	21.202	15.535	-12.379	1.00	17.48	A	O
ATOM	597	CG2	THR	A	81	23.229	14.420	-12.289	1.00	21.52	A	C
ATOM	598	C	THR	A	81	20.650	15.185	-9.470	1.00	17.64	A	C
ATOM	599	O	THR	A	81	19.466	14.858	-9.423	1.00	17.77	A	O
ATOM	600	N	ASN	A	82	21.115	16.238	-8.803	1.00	16.86	A	N
ATOM	601	CA	ASN	A	82	20.271	16.947	-7.842	1.00	16.82	A	C
ATOM	602	CB	ASN	A	82	19.279	17.840	-8.574	1.00	16.90	A	C
ATOM	603	CG	ASN	A	82	19.962	18.782	-9.552	1.00	18.05	A	C
ATOM	604	OD1	ASN	A	82	19.861	18.632	-10.804	1.00	20.14	A	O
ATOM	605	ND2	ASN	A	82	20.650	19.760	-9.005	1.00	12.31	A	N
ATOM	606	C	ASN	A	82	19.541	15.941	-6.930	1.00	16.16	A	C



ATOM	607	O	ASN	A	82	18.325	15.985	-6.772	1.00	16.88	A	O
ATOM	608	N	LYS	A	83	20.310	15.022	-6.366	1.00	15.41	A	N
ATOM	609	CA	LYS	A	83	19.767	13.853	-5.710	1.00	15.60	A	C
ATOM	610	CB	LYS	A	83	20.907	12.919	-5.287	1.00	15.95	A	C
ATOM	611	CG	LYS	A	83	21.665	12.168	-6.415	1.00	16.19	A	C
ATOM	612	CD	LYS	A	83	22.815	11.339	-5.811	1.00	19.24	A	C
ATOM	613	CE	LYS	A	83	23.806	10.791	-6.833	1.00	21.12	A	C
ATOM	614	NZ	LYS	A	83	23.076	9.941	-7.791	1.00	20.88	A	N
ATOM	615	C	LYS	A	83	18.966	14.243	-4.453	1.00	14.74	A	C
ATOM	616	O	LYS	A	83	19.243	15.248	-3.801	1.00	13.71	A	O
ATOM	617	N	GLY	A	84	18.000	13.402	-4.117	1.00	14.66	A	N
ATOM	618	CA	GLY	A	84	17.337	13.439	-2.833	1.00	14.40	A	C
ATOM	619	C	GLY	A	84	18.240	13.078	-1.664	1.00	14.38	A	C
ATOM	620	O	GLY	A	84	19.372	12.683	-1.853	1.00	14.68	A	O
ATOM	621	N	MET	A	85	17.734	13.231	-0.439	1.00	13.41	A	N
ATOM	622	CA	MET	A	85	18.586	13.079	0.753	1.00	13.39	A	C
ATOM	623	CB	MET	A	85	17.865	13.660	1.970	1.00	13.62	A	C
ATOM	624	CG	MET	A	85	17.446	15.132	1.799	1.00	14.10	A	C
ATOM	625	SD	MET	A	85	18.823	16.235	1.480	1.00	15.77	A	S
ATOM	626	CE	MET	A	85	18.801	16.373	-0.341	1.00	16.54	A	C
ATOM	627	C	MET	A	85	18.946	11.600	1.022	1.00	13.55	A	C
ATOM	628	O	MET	A	85	19.975	11.302	1.623	1.00	13.91	A	O
ATOM	629	N	ALA	A	86	18.078	10.685	0.586	1.00	13.51	A	N
ATOM	630	CA	ALA	A	86	18.290	9.250	0.774	1.00	13.69	A	C
ATOM	631	CB	ALA	A	86	17.223	8.682	1.717	1.00	13.63	A	C
ATOM	632	C	ALA	A	86	18.200	8.571	-0.589	1.00	13.59	A	C
ATOM	633	O	ALA	A	86	17.258	7.821	-0.868	1.00	14.50	A	O
ATOM	634	N	PRO	A	87	19.175	8.818	-1.445	1.00	14.33	A	N
ATOM	635	CA	PRO	A	87	19.068	8.409	-2.859	1.00	14.18	A	C
ATOM	636	CB	PRO	A	87	20.236	9.152	-3.515	1.00	14.93	A	C
ATOM	637	CG	PRO	A	87	21.263	9.267	-2.393	1.00	14.56	A	C
ATOM	638	CD	PRO	A	87	20.446	9.524	-1.148	1.00	13.97	A	C
ATOM	639	C	PRO	A	87	19.146	6.901	-3.123	1.00	14.68	A	C
ATOM	640	O	PRO	A	87	18.943	6.474	-4.260	1.00	15.65	A	O
ATOM	641	N	GLN	A	88	19.424	6.099	-2.109	1.00	15.11	A	N
ATOM	642	CA	GLN	A	88	19.436	4.639	-2.266	1.00	16.35	A	C
ATOM	643	CB	GLN	A	88	20.748	4.050	-1.733	1.00	16.73	A	C
ATOM	644	CG	GLN	A	88	21.900	4.262	-2.703	1.00	19.50	A	C
ATOM	645	CD	GLN	A	88	23.267	3.916	-2.161	1.00	21.39	A	C
ATOM	646	OE1	GLN	A	88	23.427	2.933	-1.439	1.00	22.79	A	O
ATOM	647	NE2	GLN	A	88	24.272	4.709	-2.547	1.00	22.41	A	N
ATOM	648	C	GLN	A	88	18.228	3.976	-1.621	1.00	16.49	A	C
ATOM	649	O	GLN	A	88	18.080	2.754	-1.644	1.00	16.50	A	O
ATOM	650	N	ALA	A	89	17.347	4.786	-1.044	1.00	16.72	A	N
ATOM	651	CA	ALA	A	89	16.056	4.279	-0.599	1.00	16.78	A	C
ATOM	652	CB	ALA	A	89	15.380	5.277	0.375	1.00	17.28	A	C
ATOM	653	C	ALA	A	89	15.139	3.996	-1.792	1.00	16.32	A	C
ATOM	654	O	ALA	A	89	15.212	4.648	-2.826	1.00	16.81	A	O
ATOM	655	N	ASN	A	90	14.248	3.037	-1.634	1.00	15.45	A	N
ATOM	656	CA	ASN	A	90	13.264	2.756	-2.658	1.00	15.40	A	C
ATOM	657	CB	ASN	A	90	13.036	1.247	-2.756	1.00	16.05	A	C
ATOM	658	CG	ASN	A	90	14.076	0.549	-3.658	1.00	19.92	A	C
ATOM	659	OD1	ASN	A	90	15.039	1.155	-4.106	1.00	25.00	A	O
ATOM	660	ND2	ASN	A	90	13.892	-0.736	-3.873	1.00	28.28	A	N
ATOM	661	C	ASN	A	90	11.942	3.486	-2.367	1.00	14.01	A	C
ATOM	662	O	ASN	A	90	11.668	3.834	-1.234	1.00	12.81	A	O
ATOM	663	N	LEU	A	91	11.150	3.705	-3.410	1.00	13.02	A	N
ATOM	664	CA	LEU	A	91	9.964	4.542	-3.381	1.00	13.78	A	C

ATOM	665	CB	LEU	A	91	10.022	5.524	-4.540	1.00	13.95	A	C
ATOM	666	CG	LEU	A	91	8.861	6.472	-4.765	1.00	12.85	A	C
ATOM	667	CD1	LEU	A	91	8.669	7.375	-3.571	1.00	15.80	A	C
ATOM	668	CD2	LEU	A	91	9.077	7.287	-6.026	1.00	13.13	A	C
ATOM	669	C	LEU	A	91	8.661	3.762	-3.524	1.00	14.15	A	C
ATOM	670	O	LEU	A	91	8.503	2.953	-4.437	1.00	15.63	A	O
ATOM	671	N	VAL	A	92	7.716	4.055	-2.649	1.00	13.69	A	N
ATOM	672	CA	VAL	A	92	6.327	3.692	-2.872	1.00	14.00	A	C
ATOM	673	CB	VAL	A	92	5.737	3.031	-1.662	1.00	13.15	A	C
ATOM	674	CG1	VAL	A	92	4.197	3.018	-1.767	1.00	15.32	A	C
ATOM	675	CG2	VAL	A	92	6.260	1.621	-1.546	1.00	13.02	A	C
ATOM	676	C	VAL	A	92	5.615	5.001	-3.175	1.00	13.45	A	C
ATOM	677	O	VAL	A	92	5.687	5.942	-2.376	1.00	13.53	A	O
ATOM	678	N	PHE	A	93	4.984	5.107	-4.346	1.00	13.19	A	N
ATOM	679	CA	PHE	A	93	4.293	6.351	-4.714	1.00	13.05	A	C
ATOM	680	CB	PHE	A	93	4.899	6.964	-5.985	1.00	13.57	A	C
ATOM	681	CG	PHE	A	93	4.484	8.388	-6.206	1.00	13.50	A	C
ATOM	682	CD1	PHE	A	93	5.331	9.439	-5.861	1.00	13.00	A	C
ATOM	683	CE1	PHE	A	93	4.941	10.748	-6.023	1.00	12.71	A	C
ATOM	684	CZ	PHE	A	93	3.680	11.030	-6.515	1.00	11.77	A	C
ATOM	685	CE2	PHE	A	93	2.832	9.998	-6.881	1.00	12.22	A	C
ATOM	686	CD2	PHE	A	93	3.226	8.679	-6.710	1.00	12.44	A	C
ATOM	687	C	PHE	A	93	2.793	6.150	-4.872	1.00	13.51	A	C
ATOM	688	O	PHE	A	93	2.350	5.285	-5.632	1.00	13.61	A	O
ATOM	689	N	GLN	A	94	2.021	6.949	-4.150	1.00	13.35	A	N
ATOM	690	CA	GLN	A	94	0.567	6.903	-4.197	1.00	13.55	A	C
ATOM	691	CB	GLN	A	94	-0.034	6.775	-2.786	1.00	12.95	A	C
ATOM	692	CG	GLN	A	94	0.383	5.493	-2.078	1.00	13.25	A	C
ATOM	693	CD	GLN	A	94	0.065	5.494	-0.589	1.00	14.07	A	C
ATOM	694	OE1	GLN	A	94	0.598	6.311	0.157	1.00	16.83	A	O
ATOM	695	NE2	GLN	A	94	-0.813	4.578	-0.158	1.00	13.83	A	N
ATOM	696	C	GLN	A	94	0.118	8.195	-4.841	1.00	13.81	A	C
ATOM	697	O	GLN	A	94	0.197	9.289	-4.236	1.00	12.11	A	O
ATOM	698	N	SER	A	95	-0.266	8.072	-6.110	1.00	14.33	A	N
ATOM	699	CA	SER	A	95	-0.793	9.190	-6.893	1.00	14.08	A	C
ATOM	700	CB	SER	A	95	-0.743	8.850	-8.380	1.00	13.95	A	C
ATOM	701	OG	SER	A	95	-1.337	9.864	-9.152	1.00	11.92	A	O
ATOM	702	C	SER	A	95	-2.221	9.519	-6.494	1.00	14.82	A	C
ATOM	703	O	SER	A	95	-3.150	8.743	-6.780	1.00	14.73	A	O
ATOM	704	N	ILE	A	96	-2.404	10.681	-5.852	1.00	15.21	A	N
ATOM	705	CA	ILE	A	96	-3.699	11.049	-5.277	1.00	15.55	A	C
ATOM	706	CB	ILE	A	96	-3.560	11.482	-3.782	1.00	15.92	A	C
ATOM	707	CG1	ILE	A	96	-2.466	12.548	-3.597	1.00	16.08	A	C
ATOM	708	CD1	ILE	A	96	-2.367	13.122	-2.196	1.00	17.02	A	C
ATOM	709	CG2	ILE	A	96	-3.257	10.273	-2.915	1.00	16.70	A	C
ATOM	710	C	ILE	A	96	-4.398	12.158	-6.043	1.00	15.93	A	C
ATOM	711	O	ILE	A	96	-5.475	12.590	-5.660	1.00	14.84	A	O
ATOM	712	N	MET	A	97	-3.797	12.640	-7.119	1.00	16.32	A	N
ATOM	713	CA	MET	A	97	-4.440	13.700	-7.889	1.00	18.17	A	C
ATOM	714	CB	MET	A	97	-3.471	14.346	-8.884	1.00	18.20	A	C
ATOM	715	CG	MET	A	97	-4.107	15.480	-9.688	1.00	21.58	A	C
ATOM	716	SD	MET	A	97	-2.949	16.297	-10.814	1.00	25.41	A	S
ATOM	717	CE	MET	A	97	-3.900	16.196	-12.225	1.00	31.75	A	C
ATOM	718	C	MET	A	97	-5.647	13.114	-8.641	1.00	18.32	A	C
ATOM	719	O	MET	A	97	-5.537	12.054	-9.249	1.00	18.26	A	O
ATOM	720	N	ASP	A	98	-6.780	13.807	-8.568	1.00	19.35	A	N
ATOM	721	CA	ASP	A	98	-8.020	13.369	-9.217	1.00	20.45	A	C
ATOM	722	CB	ASP	A	98	-9.268	13.714	-8.375	1.00	20.39	A	C

ATOM	723	CG	ASP	A	98	-9.367	15.170	-8.021	1.00	21.41	A	C
ATOM	724	OD1	ASP	A	98	-9.234	16.024	-8.928	1.00	22.52	A	O
ATOM	725	OD2	ASP	A	98	-9.599	15.575	-6.847	1.00	20.32	A	O
ATOM	726	C	ASP	A	98	-8.093	14.004	-10.592	1.00	20.49	A	C
ATOM	727	O	ASP	A	98	-7.168	14.690	-10.996	1.00	19.61	A	O
ATOM	728	N	SER	A	99	-9.170	13.747	-11.321	1.00	21.70	A	N
ATOM	729	CA	SER	A	99	-9.252	14.202	-12.703	1.00	23.74	A	C
ATOM	730	CB	SER	A	99	-10.202	13.301	-13.510	1.00	24.07	A	C
ATOM	731	OG	SER	A	99	-11.497	13.436	-12.986	1.00	25.19	A	O
ATOM	732	C	SER	A	99	-9.727	15.660	-12.749	1.00	24.80	A	C
ATOM	733	O	SER	A	99	-9.696	16.286	-13.812	1.00	27.46	A	O
ATOM	734	N	GLY	A	100	-10.152	16.203	-11.611	1.00	24.38	A	N
ATOM	735	CA	GLY	A	100	-10.425	17.621	-11.488	1.00	25.17	A	C
ATOM	736	C	GLY	A	100	-9.262	18.470	-10.968	1.00	25.36	A	C
ATOM	737	O	GLY	A	100	-9.475	19.606	-10.557	1.00	26.29	A	O
ATOM	738	N	GLY	A	101	-8.047	17.933	-10.964	1.00	25.13	A	N
ATOM	739	CA	GLY	A	101	-6.873	18.715	-10.573	1.00	24.90	A	C
ATOM	740	C	GLY	A	101	-6.541	18.760	-9.076	1.00	24.55	A	C
ATOM	741	O	GLY	A	101	-5.425	19.133	-8.713	1.00	26.15	A	O
ATOM	742	N	GLY	A	102	-7.490	18.406	-8.221	1.00	22.32	A	N
ATOM	743	CA	GLY	A	102	-7.258	18.339	-6.783	1.00	21.84	A	C
ATOM	744	C	GLY	A	102	-6.703	17.008	-6.267	1.00	20.73	A	C
ATOM	745	O	GLY	A	102	-6.172	16.204	-7.021	1.00	19.11	A	O
ATOM	746	N	LEU	A	103	-6.814	16.794	-4.959	1.00	19.97	A	N
ATOM	747	CA	LEU	A	103	-6.225	15.634	-4.294	1.00	19.19	A	C
ATOM	748	CB	LEU	A	103	-5.346	16.094	-3.131	1.00	18.87	A	C
ATOM	749	CG	LEU	A	103	-4.169	16.986	-3.552	1.00	18.31	A	C
ATOM	750	CD1	LEU	A	103	-3.298	17.397	-2.354	1.00	17.54	A	C
ATOM	751	CD2	LEU	A	103	-3.341	16.297	-4.607	1.00	19.64	A	C
ATOM	752	C	LEU	A	103	-7.307	14.676	-3.809	1.00	19.31	A	C
ATOM	753	O	LEU	A	103	-7.179	14.018	-2.750	1.00	18.44	A	O
ATOM	754	N	GLY	A	104	-8.371	14.586	-4.604	1.00	18.93	A	N
ATOM	755	CA	GLY	A	104	-9.537	13.780	-4.260	1.00	18.78	A	C
ATOM	756	C	GLY	A	104	-9.259	12.298	-4.234	1.00	18.26	A	C
ATOM	757	O	GLY	A	104	-10.078	11.506	-3.780	1.00	19.17	A	O
ATOM	758	N	GLY	A	105	-8.094	11.886	-4.703	1.00	17.54	A	N
ATOM	759	CA	GLY	A	105	-7.698	10.500	-4.520	1.00	17.23	A	C
ATOM	760	C	GLY	A	105	-7.395	10.091	-3.075	1.00	16.85	A	C
ATOM	761	O	GLY	A	105	-7.319	8.895	-2.731	1.00	15.88	A	O
ATOM	762	N	LEU	A	106	-7.263	11.067	-2.194	1.00	16.62	A	N
ATOM	763	CA	LEU	A	106	-7.137	10.729	-0.777	1.00	16.79	A	C
ATOM	764	CB	LEU	A	106	-6.892	11.975	0.048	1.00	16.05	A	C
ATOM	765	CG	LEU	A	106	-5.519	12.560	-0.204	1.00	14.68	A	C
ATOM	766	CD1	LEU	A	106	-5.479	13.986	0.274	1.00	16.20	A	C
ATOM	767	CD2	LEU	A	106	-4.425	11.707	0.507	1.00	13.15	A	C
ATOM	768	C	LEU	A	106	-8.423	10.056	-0.304	1.00	17.90	A	C
ATOM	769	O	LEU	A	106	-9.513	10.553	-0.587	1.00	18.63	A	O
ATOM	770	N	PRO	A	107	-8.318	8.932	0.387	1.00	18.42	A	N
ATOM	771	CA	PRO	A	107	-9.506	8.280	0.977	1.00	19.35	A	C
ATOM	772	CB	PRO	A	107	-8.963	6.932	1.430	1.00	19.15	A	C
ATOM	773	CG	PRO	A	107	-7.537	7.286	1.774	1.00	19.19	A	C
ATOM	774	CD	PRO	A	107	-7.089	8.162	0.640	1.00	18.63	A	C
ATOM	775	C	PRO	A	107	-10.070	9.036	2.178	1.00	18.88	A	C
ATOM	776	O	PRO	A	107	-9.340	9.724	2.886	1.00	19.33	A	O
ATOM	777	N	ALA	A	108	-11.367	8.910	2.408	1.00	19.46	A	N
ATOM	778	CA	ALA	A	108	-12.022	9.562	3.530	1.00	19.50	A	C
ATOM	779	CB	ALA	A	108	-13.514	9.168	3.585	1.00	20.76	A	C
ATOM	780	C	ALA	A	108	-11.359	9.229	4.875	1.00	18.72	A	C

ATOM	781	O	ALA	A	108	-11.229	10.093	5.727	1.00	19.17	A	O
ATOM	782	N	ASN	A	109	-11.007	7.964	5.069	1.00	18.94	A	N
ATOM	783	CA	ASN	A	109	-10.193	7.535	6.209	1.00	19.10	A	C
ATOM	784	CB	ASN	A	109	-10.691	6.206	6.773	1.00	19.41	A	C
ATOM	785	CG	ASN	A	109	-9.990	5.834	8.073	1.00	22.66	A	C
ATOM	786	OD1	ASN	A	109	-8.872	6.295	8.349	1.00	19.31	A	O
ATOM	787	ND2	ASN	A	109	-10.665	5.018	8.908	1.00	25.73	A	N
ATOM	788	C	ASN	A	109	-8.731	7.392	5.804	1.00	17.97	A	C
ATOM	789	O	ASN	A	109	-8.353	6.446	5.088	1.00	17.31	A	O
ATOM	790	N	LEU	A	110	-7.895	8.325	6.245	1.00	16.66	A	N
ATOM	791	CA	LEU	A	110	-6.489	8.277	5.862	1.00	15.50	A	C
ATOM	792	CB	LEU	A	110	-5.738	9.502	6.406	1.00	15.65	A	C
ATOM	793	CG	LEU	A	110	-6.096	10.831	5.749	1.00	13.74	A	C
ATOM	794	CD1	LEU	A	110	-5.294	11.932	6.373	1.00	16.06	A	C
ATOM	795	CD2	LEU	A	110	-5.873	10.768	4.256	1.00	13.53	A	C
ATOM	796	C	LEU	A	110	-5.784	7.006	6.285	1.00	15.96	A	C
ATOM	797	O	LEU	A	110	-4.750	6.660	5.719	1.00	16.04	A	O
ATOM	798	N	GLN	A	111	-6.297	6.283	7.276	1.00	16.18	A	N
ATOM	799	CA	GLN	A	111	-5.635	5.034	7.655	1.00	16.61	A	C
ATOM	800	CB	GLN	A	111	-6.317	4.377	8.871	1.00	17.82	A	C
ATOM	801	CG	GLN	A	111	-6.337	5.320	10.077	1.00	17.25	A	C
ATOM	802	CD	GLN	A	111	-6.584	4.625	11.399	1.00	20.40	A	C
ATOM	803	OE1	GLN	A	111	-5.934	3.635	11.699	1.00	21.99	A	O
ATOM	804	NE2	GLN	A	111	-7.513	5.163	12.202	1.00	19.23	A	N
ATOM	805	C	GLN	A	111	-5.560	4.086	6.461	1.00	17.45	A	C
ATOM	806	O	GLN	A	111	-4.601	3.323	6.312	1.00	17.74	A	O
ATOM	807	N	THR	A	112	-6.522	4.195	5.548	1.00	16.47	A	N
ATOM	808	CA	THR	A	112	-6.483	3.418	4.309	1.00	16.12	A	C
ATOM	809	CB	THR	A	112	-7.756	3.733	3.510	1.00	16.21	A	C
ATOM	810	OG1	THR	A	112	-8.900	3.480	4.333	1.00	17.07	A	O
ATOM	811	CG2	THR	A	112	-7.909	2.838	2.305	1.00	16.70	A	C
ATOM	812	C	THR	A	112	-5.252	3.711	3.442	1.00	15.86	A	C
ATOM	813	O	THR	A	112	-4.623	2.789	2.869	1.00	15.50	A	O
ATOM	814	N	LEU	A	113	-4.933	4.995	3.303	1.00	14.75	A	N
ATOM	815	CA	LEU	A	113	-3.742	5.413	2.558	1.00	14.05	A	C
ATOM	816	CB	LEU	A	113	-3.677	6.941	2.557	1.00	14.27	A	C
ATOM	817	CG	LEU	A	113	-2.549	7.597	1.807	1.00	14.53	A	C
ATOM	818	CD1	LEU	A	113	-2.840	7.473	0.297	1.00	16.65	A	C
ATOM	819	CD2	LEU	A	113	-2.412	9.039	2.212	1.00	13.95	A	C
ATOM	820	C	LEU	A	113	-2.478	4.836	3.212	1.00	13.77	A	C
ATOM	821	O	LEU	A	113	-1.625	4.238	2.550	1.00	13.55	A	O
ATOM	822	N	PHE	A	114	-2.361	5.016	4.523	1.00	12.95	A	N
ATOM	823	CA	PHE	A	114	-1.182	4.528	5.223	1.00	13.04	A	C
ATOM	824	CB	PHE	A	114	-1.154	5.049	6.645	1.00	12.56	A	C
ATOM	825	CG	PHE	A	114	-1.331	6.551	6.743	1.00	11.79	A	C
ATOM	826	CD1	PHE	A	114	-0.639	7.402	5.902	1.00	12.07	A	C
ATOM	827	CE1	PHE	A	114	-0.785	8.781	5.986	1.00	12.47	A	C
ATOM	828	CZ	PHE	A	114	-1.662	9.323	6.921	1.00	13.57	A	C
ATOM	829	CE2	PHE	A	114	-2.365	8.470	7.754	1.00	11.94	A	C
ATOM	830	CD2	PHE	A	114	-2.186	7.100	7.663	1.00	9.85	A	C
ATOM	831	C	PHE	A	114	-1.060	3.003	5.171	1.00	13.86	A	C
ATOM	832	O	PHE	A	114	0.063	2.461	5.004	1.00	12.73	A	O
ATOM	833	N	SER	A	115	-2.196	2.306	5.277	1.00	14.04	A	N
ATOM	834	CA	SER	A	115	-2.148	0.848	5.292	1.00	14.17	A	C
ATOM	835	CB	BSER	A	115	-3.527	0.252	5.640	0.50	13.81	A	C
ATOM	836	CB	ASER	A	115	-3.457	0.215	5.769	0.50	14.55	A	C
ATOM	837	OG	BSER	A	115	-3.970	0.566	6.958	0.50	10.51	A	O
ATOM	838	OG	ASER	A	115	-4.544	0.608	4.978	0.50	18.03	A	O



ATOM	839	C	SER	A	115	-1.677	0.296	3.943	1.00	14.11	A	C
ATOM	840	O	SER	A	115	-0.932	-0.663	3.909	1.00	13.43	A	O
ATOM	841	N	GLN	A	116	-2.108	0.890	2.832	1.00	14.73	A	N
ATOM	842	CA	GLN	A	116	-1.656	0.442	1.513	1.00	14.53	A	C
ATOM	843	CB	GLN	A	116	-2.394	1.234	0.417	1.00	15.81	A	C
ATOM	844	CG	GLN	A	116	-1.947	0.951	-1.038	1.00	15.88	A	C
ATOM	845	CD	GLN	A	116	-2.601	1.886	-2.007	1.00	16.75	A	C
ATOM	846	OE1	GLN	A	116	-2.629	3.086	-1.747	1.00	14.56	A	O
ATOM	847	NE2	GLN	A	116	-3.200	1.346	-3.106	1.00	14.07	A	N
ATOM	848	C	GLN	A	116	-0.131	0.571	1.375	1.00	14.16	A	C
ATOM	849	O	GLN	A	116	0.554	-0.336	0.861	1.00	14.37	A	O
ATOM	850	N	ALA	A	117	0.407	1.679	1.862	1.00	13.34	A	N
ATOM	851	CA	ALA	A	117	1.838	1.930	1.795	1.00	13.79	A	C
ATOM	852	CB	ALA	A	117	2.152	3.408	2.151	1.00	13.52	A	C
ATOM	853	C	ALA	A	117	2.608	0.972	2.714	1.00	13.17	A	C
ATOM	854	O	ALA	A	117	3.666	0.472	2.344	1.00	13.07	A	O
ATOM	855	N	TYR	A	118	2.071	0.740	3.908	1.00	13.32	A	N
ATOM	856	CA	TYR	A	118	2.679	-0.161	4.877	1.00	13.82	A	C
ATOM	857	CB	TYR	A	118	1.878	-0.177	6.190	1.00	14.02	A	C
ATOM	858	CG	TYR	A	118	2.636	-0.861	7.324	1.00	17.04	A	C
ATOM	859	CD1	TYR	A	118	2.472	-2.216	7.589	1.00	20.14	A	C
ATOM	860	CE1	TYR	A	118	3.186	-2.839	8.640	1.00	24.14	A	C
ATOM	861	CZ	TYR	A	118	4.041	-2.071	9.409	1.00	23.61	A	C
ATOM	862	OH	TYR	A	118	4.762	-2.631	10.442	1.00	28.49	A	O
ATOM	863	CE2	TYR	A	118	4.194	-0.725	9.155	1.00	20.69	A	C
ATOM	864	CD2	TYR	A	118	3.501	-0.135	8.136	1.00	18.61	A	C
ATOM	865	C	TYR	A	118	2.782	-1.576	4.294	1.00	14.18	A	C
ATOM	866	O	TYR	A	118	3.838	-2.228	4.363	1.00	14.05	A	O
ATOM	867	N	SER	A	119	1.705	-2.024	3.669	1.00	14.24	A	N
ATOM	868	CA	SER	A	119	1.684	-3.358	3.064	1.00	15.13	A	C
ATOM	869	CB	SER	A	119	0.288	-3.660	2.544	1.00	14.77	A	C
ATOM	870	OG	SER	A	119	-0.609	-3.744	3.638	1.00	13.56	A	O
ATOM	871	C	SER	A	119	2.752	-3.531	1.977	1.00	15.67	A	C
ATOM	872	O	SER	A	119	3.313	-4.602	1.818	1.00	15.80	A	O
ATOM	873	N	ALA	A	120	3.052	-2.461	1.254	1.00	16.24	A	N
ATOM	874	CA	ALA	A	120	4.085	-2.488	0.204	1.00	15.93	A	C
ATOM	875	CB	ALA	A	120	3.847	-1.352	-0.759	1.00	16.16	A	C
ATOM	876	C	ALA	A	120	5.504	-2.405	0.767	1.00	16.13	A	C
ATOM	877	O	ALA	A	120	6.474	-2.473	0.030	1.00	16.93	A	O
ATOM	878	N	GLY	A	121	5.626	-2.249	2.083	1.00	16.23	A	N
ATOM	879	CA	GLY	A	121	6.917	-2.249	2.747	1.00	15.35	A	C
ATOM	880	C	GLY	A	121	7.400	-0.883	3.247	1.00	15.15	A	C
ATOM	881	O	GLY	A	121	8.466	-0.811	3.893	1.00	15.57	A	O
ATOM	882	N	ALA	A	122	6.665	0.195	2.977	1.00	14.40	A	N
ATOM	883	CA	ALA	A	122	7.110	1.522	3.443	1.00	14.85	A	C
ATOM	884	CB	ALA	A	122	6.273	2.632	2.831	1.00	14.84	A	C
ATOM	885	C	ALA	A	122	7.057	1.635	4.964	1.00	14.35	A	C
ATOM	886	O	ALA	A	122	6.078	1.230	5.574	1.00	15.21	A	O
ATOM	887	N	ARG	A	123	8.077	2.223	5.570	1.00	13.62	A	N
ATOM	888	CA	ARG	A	123	8.013	2.499	7.008	1.00	12.85	A	C
ATOM	889	CB	ARG	A	123	9.065	1.689	7.761	1.00	12.85	A	C
ATOM	890	CG	ARG	A	123	8.870	0.162	7.597	1.00	13.74	A	C
ATOM	891	CD	ARG	A	123	7.584	-0.334	8.290	1.00	14.35	A	C
ATOM	892	NE	ARG	A	123	7.396	-1.786	8.187	1.00	14.77	A	N
ATOM	893	CZ	ARG	A	123	6.676	-2.389	7.253	1.00	16.63	A	C
ATOM	894	NH1	ARG	A	123	6.039	-1.678	6.337	1.00	15.68	A	N
ATOM	895	NH2	ARG	A	123	6.579	-3.719	7.240	1.00	17.36	A	N
ATOM	896	C	ARG	A	123	8.132	3.987	7.298	1.00	12.72	A	C



ATOM	897	O	ARG	A	123	8.116	4.418	8.448	1.00	12.15	A	O
ATOM	898	N	ILE	A	124	8.225	4.773	6.234	1.00	12.67	A	N
ATOM	899	CA	ILE	A	124	8.177	6.218	6.346	1.00	12.97	A	C
ATOM	900	CB	ILE	A	124	9.554	6.814	6.025	1.00	12.64	A	C
ATOM	901	CG1	ILE	A	124	10.619	6.262	6.985	1.00	13.71	A	C
ATOM	902	CD1	ILE	A	124	12.068	6.395	6.480	1.00	14.82	A	C
ATOM	903	CG2	ILE	A	124	9.478	8.348	6.061	1.00	13.97	A	C
ATOM	904	C	ILE	A	124	7.160	6.695	5.324	1.00	12.91	A	C
ATOM	905	O	ILE	A	124	7.132	6.195	4.210	1.00	13.07	A	O
ATOM	906	N	HIS	A	125	6.365	7.696	5.671	1.00	12.94	A	N
ATOM	907	CA	HIS	A	125	5.252	8.100	4.823	1.00	12.77	A	C
ATOM	908	CB	HIS	A	125	3.894	7.549	5.353	1.00	13.00	A	C
ATOM	909	CG	HIS	A	125	2.806	7.650	4.334	1.00	15.91	A	C
ATOM	910	ND1	HIS	A	125	2.428	8.850	3.783	1.00	13.47	A	N
ATOM	911	CE1	HIS	A	125	1.547	8.632	2.821	1.00	16.40	A	C
ATOM	912	NE2	HIS	A	125	1.312	7.333	2.756	1.00	16.49	A	N
ATOM	913	CD2	HIS	A	125	2.072	6.699	3.705	1.00	18.35	A	C
ATOM	914	C	HIS	A	125	5.223	9.620	4.828	1.00	12.62	A	C
ATOM	915	O	HIS	A	125	5.053	10.202	5.893	1.00	12.04	A	O
ATOM	916	N	THR	A	126	5.401	10.268	3.674	1.00	12.71	A	N
ATOM	917	CA	THR	A	126	5.527	11.738	3.641	1.00	12.63	A	C
ATOM	918	CB	THR	A	126	6.984	12.142	3.302	1.00	12.63	A	C
ATOM	919	OG1	THR	A	126	7.121	13.560	3.334	1.00	12.18	A	O
ATOM	920	CG2	THR	A	126	7.395	11.747	1.864	1.00	12.36	A	C
ATOM	921	C	THR	A	126	4.498	12.426	2.735	1.00	12.60	A	C
ATOM	922	O	THR	A	126	4.166	11.931	1.652	1.00	12.62	A	O
ATOM	923	N	ASN	A	127	4.010	13.572	3.200	1.00	12.52	A	N
ATOM	924	CA	ASN	A	127	2.778	14.189	2.696	1.00	12.84	A	C
ATOM	925	CB	ASN	A	127	1.599	13.811	3.605	1.00	13.04	A	C
ATOM	926	CG	ASN	A	127	1.433	12.325	3.720	1.00	13.25	A	C
ATOM	927	OD1	ASN	A	127	1.916	11.686	4.690	1.00	13.15	A	O
ATOM	928	ND2	ASN	A	127	0.814	11.740	2.712	1.00	9.82	A	N
ATOM	929	C	ASN	A	127	2.894	15.706	2.637	1.00	12.70	A	C
ATOM	930	O	ASN	A	127	2.798	16.390	3.661	1.00	13.27	A	O
ATOM	931	N	SER	A	128	3.103	16.211	1.435	1.00	12.76	A	N
ATOM	932	CA	SER	A	128	3.277	17.640	1.162	1.00	13.02	A	C
ATOM	933	CB	SER	A	128	4.308	17.831	0.043	1.00	12.57	A	C
ATOM	934	OG	SER	A	128	5.608	17.510	0.485	1.00	12.52	A	O
ATOM	935	C	SER	A	128	1.927	18.238	0.748	1.00	13.42	A	C
ATOM	936	O	SER	A	128	1.763	18.767	-0.372	1.00	13.82	A	O
ATOM	937	N	TRP	A	129	0.968	18.129	1.663	1.00	13.86	A	N
ATOM	938	CA	TRP	A	129	-0.392	18.616	1.465	1.00	13.67	A	C
ATOM	939	CB	TRP	A	129	-1.215	17.648	0.602	1.00	13.88	A	C
ATOM	940	CG	TRP	A	129	-1.130	16.180	0.964	1.00	13.08	A	C
ATOM	941	CD1	TRP	A	129	-0.305	15.232	0.391	1.00	14.80	A	C
ATOM	942	NE1	TRP	A	129	-0.531	13.997	0.956	1.00	12.40	A	N
ATOM	943	CE2	TRP	A	129	-1.518	14.122	1.900	1.00	13.40	A	C
ATOM	944	CD2	TRP	A	129	-1.924	15.480	1.921	1.00	12.64	A	C
ATOM	945	CE3	TRP	A	129	-2.948	15.857	2.806	1.00	14.15	A	C
ATOM	946	CZ3	TRP	A	129	-3.504	14.910	3.614	1.00	13.25	A	C
ATOM	947	CH2	TRP	A	129	-3.082	13.566	3.559	1.00	13.78	A	C
ATOM	948	CZ2	TRP	A	129	-2.101	13.158	2.711	1.00	12.56	A	C
ATOM	949	C	TRP	A	129	-1.089	18.859	2.782	1.00	14.44	A	C
ATOM	950	O	TRP	A	129	-0.612	18.460	3.876	1.00	14.19	A	O
ATOM	951	N	GLY	A	130	-2.224	19.538	2.694	1.00	14.75	A	N
ATOM	952	CA	GLY	A	130	-3.004	19.834	3.866	1.00	15.45	A	C
ATOM	953	C	GLY	A	130	-4.173	20.744	3.563	1.00	16.66	A	C
ATOM	954	O	GLY	A	130	-4.203	21.394	2.518	1.00	16.04	A	O

ATOM	955	N	ALA	A	131	-5.139	20.754	4.478	1.00	16.87	A	N
ATOM	956	CA	ALA	A	131	-6.222	21.733	4.484	1.00	18.19	A	C
ATOM	957	CB	ALA	A	131	-7.515	21.097	4.983	1.00	17.33	A	C
ATOM	958	C	ALA	A	131	-5.843	22.852	5.423	1.00	19.54	A	C
ATOM	959	O	ALA	A	131	-5.562	22.590	6.592	1.00	20.18	A	O
ATOM	960	N	PRO	A	132	-5.869	24.090	4.942	1.00	20.97	A	N
ATOM	961	CA	PRO	A	132	-5.513	25.253	5.763	1.00	21.46	A	C
ATOM	962	CB	PRO	A	132	-5.260	26.346	4.724	1.00	21.95	A	C
ATOM	963	CG	PRO	A	132	-6.060	25.967	3.546	1.00	22.18	A	C
ATOM	964	CD	PRO	A	132	-6.220	24.462	3.564	1.00	21.43	A	C
ATOM	965	C	PRO	A	132	-6.595	25.676	6.753	1.00	22.74	A	C
ATOM	966	O	PRO	A	132	-7.272	26.703	6.555	1.00	24.13	A	O
ATOM	967	N	VAL	A	133	-6.708	24.912	7.833	1.00	22.71	A	N
ATOM	968	CA	VAL	A	133	-7.723	25.086	8.850	1.00	23.39	A	C
ATOM	969	CB	VAL	A	133	-8.349	23.712	9.223	1.00	23.48	A	C
ATOM	970	CG1	VAL	A	133	-9.115	23.133	8.045	1.00	25.68	A	C
ATOM	971	CG2	VAL	A	133	-7.269	22.750	9.687	1.00	24.53	A	C
ATOM	972	C	VAL	A	133	-7.223	25.742	10.150	1.00	23.23	A	C
ATOM	973	O	VAL	A	133	-7.855	25.599	11.185	1.00	22.57	A	O
ATOM	974	N	ASN	A	134	-6.094	26.437	10.098	1.00	23.10	A	N
ATOM	975	CA	ASN	A	134	-5.660	27.279	11.201	1.00	23.36	A	C
ATOM	976	CB	ASN	A	134	-6.583	28.512	11.310	1.00	24.40	A	C
ATOM	977	CG	ASN	A	134	-6.491	29.413	10.082	1.00	26.68	A	C
ATOM	978	OD1	ASN	A	134	-7.489	30.000	9.650	1.00	34.40	A	O
ATOM	979	ND2	ASN	A	134	-5.315	29.478	9.482	1.00	28.87	A	N
ATOM	980	C	ASN	A	134	-5.588	26.561	12.535	1.00	22.43	A	C
ATOM	981	O	ASN	A	134	-6.210	26.971	13.510	1.00	21.30	A	O
ATOM	982	N	GLY	A	135	-4.844	25.458	12.574	1.00	21.06	A	N
ATOM	983	CA	GLY	A	135	-4.548	24.840	13.846	1.00	20.36	A	C
ATOM	984	C	GLY	A	135	-5.541	23.818	14.308	1.00	19.66	A	C
ATOM	985	O	GLY	A	135	-5.320	23.200	15.327	1.00	18.95	A	O
ATOM	986	N	ALA	A	136	-6.613	23.595	13.557	1.00	19.08	A	N
ATOM	987	CA	ALA	A	136	-7.609	22.643	14.006	1.00	19.00	A	C
ATOM	988	CB	ALA	A	136	-8.925	22.778	13.199	1.00	19.34	A	C
ATOM	989	C	ALA	A	136	-7.098	21.206	13.893	1.00	19.31	A	C
ATOM	990	O	ALA	A	136	-6.354	20.851	12.952	1.00	18.44	A	O
ATOM	991	N	TYR	A	137	-7.568	20.407	14.841	1.00	18.56	A	N
ATOM	992	CA	TYR	A	137	-7.341	18.979	14.907	1.00	18.99	A	C
ATOM	993	CB	TYR	A	137	-7.112	18.588	16.367	1.00	18.67	A	C
ATOM	994	CG	TYR	A	137	-6.637	17.175	16.588	1.00	19.68	A	C
ATOM	995	CD1	TYR	A	137	-7.537	16.173	16.885	1.00	19.55	A	C
ATOM	996	CE1	TYR	A	137	-7.112	14.855	17.099	1.00	21.07	A	C
ATOM	997	CZ	TYR	A	137	-5.765	14.548	17.045	1.00	20.92	A	C
ATOM	998	OH	TYR	A	137	-5.371	13.250	17.265	1.00	20.20	A	O
ATOM	999	CE2	TYR	A	137	-4.837	15.538	16.754	1.00	20.35	A	C
ATOM	1000	CD2	TYR	A	137	-5.278	16.848	16.522	1.00	19.75	A	C
ATOM	1001	C	TYR	A	137	-8.600	18.314	14.337	1.00	18.91	A	C
ATOM	1002	O	TYR	A	137	-9.648	18.229	14.994	1.00	18.41	A	O
ATOM	1003	N	THR	A	138	-8.481	17.872	13.091	1.00	18.62	A	N
ATOM	1004	CA	THR	A	138	-9.608	17.401	12.329	1.00	17.86	A	C
ATOM	1005	CB	THR	A	138	-9.480	17.836	10.897	1.00	18.02	A	C
ATOM	1006	OG1	THR	A	138	-8.271	17.308	10.321	1.00	16.63	A	O
ATOM	1007	CG2	THR	A	138	-9.308	19.330	10.788	1.00	17.63	A	C
ATOM	1008	C	THR	A	138	-9.593	15.888	12.407	1.00	18.43	A	C
ATOM	1009	O	THR	A	138	-8.662	15.296	12.954	1.00	17.82	A	O
ATOM	1010	N	THR	A	139	-10.624	15.278	11.843	1.00	18.06	A	N
ATOM	1011	CA	THR	A	139	-10.713	13.843	11.705	1.00	17.69	A	C
ATOM	1012	CB	THR	A	139	-12.020	13.472	10.947	1.00	18.57	A	C

ATOM	1013	OG1	THR	A	139	-13.162	13.907	11.705	1.00	20.05	A	O
ATOM	1014	CG2	THR	A	139	-12.173	11.933	10.828	1.00	19.16	A	C
ATOM	1015	C	THR	A	139	-9.496	13.285	10.989	1.00	16.78	A	C
ATOM	1016	O	THR	A	139	-9.037	12.183	11.307	1.00	17.05	A	O
ATOM	1017	N	ASP	A	140	-8.976	14.002	10.002	1.00	15.81	A	N
ATOM	1018	CA	ASP	A	140	-7.758	13.544	9.351	1.00	15.65	A	C
ATOM	1019	CB	ASP	A	140	-7.391	14.429	8.177	1.00	15.45	A	C
ATOM	1020	CG	ASP	A	140	-8.279	14.209	6.984	1.00	16.65	A	C
ATOM	1021	OD1	ASP	A	140	-8.495	15.189	6.263	1.00	18.76	A	O
ATOM	1022	OD2	ASP	A	140	-8.781	13.102	6.702	1.00	16.74	A	O
ATOM	1023	C	ASP	A	140	-6.567	13.504	10.352	1.00	15.55	A	C
ATOM	1024	O	ASP	A	140	-5.823	12.532	10.395	1.00	15.72	A	O
ATOM	1025	N	SER	A	141	-6.395	14.555	11.133	1.00	15.34	A	N
ATOM	1026	CA	SER	A	141	-5.375	14.548	12.187	1.00	15.53	A	C
ATOM	1027	CB	SER	A	141	-5.428	15.823	13.006	1.00	14.57	A	C
ATOM	1028	OG	SER	A	141	-5.275	16.936	12.173	1.00	16.14	A	O
ATOM	1029	C	SER	A	141	-5.514	13.375	13.157	1.00	15.46	A	C
ATOM	1030	O	SER	A	141	-4.511	12.754	13.558	1.00	15.37	A	O
ATOM	1031	N	ARG	A	142	-6.754	13.100	13.546	1.00	15.27	A	N
ATOM	1032	CA	ARG	A	142	-7.053	11.998	14.462	1.00	15.97	A	C
ATOM	1033	CB	ARG	A	142	-8.539	12.004	14.843	1.00	16.78	A	C
ATOM	1034	CG	ARG	A	142	-8.882	11.091	16.022	1.00	18.90	A	C
ATOM	1035	CD	ARG	A	142	-10.365	11.103	16.436	1.00	22.40	A	C
ATOM	1036	NE	ARG	A	142	-10.533	10.384	17.704	1.00	25.70	A	N
ATOM	1037	CZ	ARG	A	142	-10.549	9.057	17.839	1.00	29.38	A	C
ATOM	1038	NH1	ARG	A	142	-10.423	8.249	16.786	1.00	30.26	A	N
ATOM	1039	NH2	ARG	A	142	-10.685	8.524	19.048	1.00	30.56	A	N
ATOM	1040	C	ARG	A	142	-6.703	10.643	13.860	1.00	15.43	A	C
ATOM	1041	O	ARG	A	142	-6.107	9.778	14.534	1.00	14.36	A	O
ATOM	1042	N	ASN	A	143	-7.068	10.437	12.593	1.00	14.96	A	N
ATOM	1043	CA	ASN	A	143	-6.699	9.187	11.926	1.00	14.70	A	C
ATOM	1044	CB	ASN	A	143	-7.451	9.062	10.593	1.00	15.54	A	C
ATOM	1045	CG	ASN	A	143	-8.952	8.709	10.803	1.00	16.85	A	C
ATOM	1046	OD1	ASN	A	143	-9.842	9.204	10.096	1.00	20.66	A	O
ATOM	1047	ND2	ASN	A	143	-9.206	7.828	11.746	1.00	15.73	A	N
ATOM	1048	C	ASN	A	143	-5.183	8.986	11.754	1.00	15.26	A	C
ATOM	1049	O	ASN	A	143	-4.691	7.854	11.879	1.00	15.15	A	O
ATOM	1050	N	VAL	A	144	-4.438	10.060	11.450	1.00	14.90	A	N
ATOM	1051	CA	VAL	A	144	-2.976	9.987	11.467	1.00	13.93	A	C
ATOM	1052	CB	VAL	A	144	-2.319	11.347	11.177	1.00	14.08	A	C
ATOM	1053	CG1	VAL	A	144	-0.803	11.272	11.422	1.00	12.32	A	C
ATOM	1054	CG2	VAL	A	144	-2.625	11.818	9.748	1.00	13.08	A	C
ATOM	1055	C	VAL	A	144	-2.478	9.507	12.843	1.00	14.23	A	C
ATOM	1056	O	VAL	A	144	-1.608	8.653	12.938	1.00	13.96	A	O
ATOM	1057	N	ASP	A	145	-3.021	10.077	13.916	1.00	14.48	A	N
ATOM	1058	CA	ASP	A	145	-2.548	9.745	15.256	1.00	14.49	A	C
ATOM	1059	CB	ASP	A	145	-3.123	10.711	16.249	1.00	14.81	A	C
ATOM	1060	CG	ASP	A	145	-2.406	12.033	16.218	1.00	15.70	A	C
ATOM	1061	OD1	ASP	A	145	-1.332	12.107	15.545	1.00	14.69	A	O
ATOM	1062	OD2	ASP	A	145	-2.845	13.048	16.803	1.00	14.46	A	O
ATOM	1063	C	ASP	A	145	-2.849	8.331	15.654	1.00	15.08	A	C
ATOM	1064	O	ASP	A	145	-1.999	7.622	16.183	1.00	14.89	A	O
ATOM	1065	N	ASP	A	146	-4.065	7.906	15.361	1.00	15.66	A	N
ATOM	1066	CA	ASP	A	146	-4.470	6.545	15.608	1.00	15.98	A	C
ATOM	1067	CB	ASP	A	146	-5.931	6.400	15.184	1.00	16.37	A	C
ATOM	1068	CG	ASP	A	146	-6.565	5.107	15.705	1.00	17.81	A	C
ATOM	1069	OD1	ASP	A	146	-6.337	4.735	16.879	1.00	18.17	A	O
ATOM	1070	OD2	ASP	A	146	-7.277	4.401	14.981	1.00	21.66	A	O

ATOM	1071	C	ASP	A	146	-3.562	5.571	14.849	1.00	16.07	A	C
ATOM	1072	O	ASP	A	146	-3.047	4.607	15.408	1.00	16.60	A	O
ATOM	1073	N	TYR	A	147	-3.324	5.842	13.576	1.00	15.73	A	N
ATOM	1074	CA	TYR	A	147	-2.463	4.988	12.772	1.00	15.49	A	C
ATOM	1075	CB	TYR	A	147	-2.387	5.486	11.314	1.00	15.22	A	C
ATOM	1076	CG	TYR	A	147	-1.759	4.421	10.459	1.00	16.31	A	C
ATOM	1077	CD1	TYR	A	147	-0.400	4.394	10.249	1.00	17.35	A	C
ATOM	1078	CE1	TYR	A	147	0.180	3.380	9.506	1.00	17.49	A	C
ATOM	1079	CZ	TYR	A	147	-0.599	2.364	9.004	1.00	16.46	A	C
ATOM	1080	OH	TYR	A	147	-0.022	1.354	8.281	1.00	20.80	A	O
ATOM	1081	CE2	TYR	A	147	-1.944	2.346	9.227	1.00	16.19	A	C
ATOM	1082	CD2	TYR	A	147	-2.523	3.364	9.947	1.00	16.98	A	C
ATOM	1083	C	TYR	A	147	-1.025	4.833	13.309	1.00	15.68	A	C
ATOM	1084	O	TYR	A	147	-0.491	3.719	13.385	1.00	14.79	A	O
ATOM	1085	N	VAL	A	148	-0.399	5.953	13.652	1.00	16.33	A	N
ATOM	1086	CA	VAL	A	148	0.975	5.950	14.144	1.00	16.18	A	C
ATOM	1087	CB	VAL	A	148	1.534	7.390	14.262	1.00	16.37	A	C
ATOM	1088	CG1	VAL	A	148	2.953	7.397	14.909	1.00	17.53	A	C
ATOM	1089	CG2	VAL	A	148	1.600	8.044	12.899	1.00	16.39	A	C
ATOM	1090	C	VAL	A	148	1.063	5.206	15.488	1.00	16.59	A	C
ATOM	1091	O	VAL	A	148	2.022	4.481	15.765	1.00	16.63	A	O
ATOM	1092	N	ARG	A	149	0.061	5.356	16.331	1.00	16.70	A	N
ATOM	1093	CA	ARG	A	149	0.109	4.628	17.589	1.00	18.28	A	C
ATOM	1094	CB	ARG	A	149	-0.920	5.133	18.600	1.00	18.33	A	C
ATOM	1095	CG	ARG	A	149	-0.585	4.657	20.002	1.00	19.51	A	C
ATOM	1096	CD	ARG	A	149	-1.566	5.035	21.071	1.00	20.84	A	C
ATOM	1097	NE	ARG	A	149	-0.987	4.731	22.383	1.00	22.92	A	N
ATOM	1098	CZ	ARG	A	149	-1.661	4.491	23.504	1.00	24.06	A	C
ATOM	1099	NH1	ARG	A	149	-2.985	4.521	23.538	1.00	25.69	A	N
ATOM	1100	NH2	ARG	A	149	-0.987	4.221	24.616	1.00	23.61	A	N
ATOM	1101	C	ARG	A	149	-0.035	3.126	17.382	1.00	18.63	A	C
ATOM	1102	O	ARG	A	149	0.517	2.346	18.156	1.00	18.97	A	O
ATOM	1103	N	LYS	A	150	-0.739	2.720	16.326	1.00	18.98	A	N
ATOM	1104	CA	LYS	A	150	-0.991	1.294	16.087	1.00	19.24	A	C
ATOM	1105	CB	LYS	A	150	-2.373	1.092	15.438	1.00	19.89	A	C
ATOM	1106	CG	LYS	A	150	-3.576	1.358	16.389	1.00	21.34	A	C
ATOM	1107	CD	LYS	A	150	-4.902	0.972	15.736	1.00	24.20	A	C
ATOM	1108	CE	LYS	A	150	-6.136	1.437	16.531	1.00	27.20	A	C
ATOM	1109	NZ	LYS	A	150	-7.373	1.614	15.668	1.00	30.36	A	N
ATOM	1110	C	LYS	A	150	0.123	0.622	15.250	1.00	18.99	A	C
ATOM	1111	O	LYS	A	150	0.296	-0.577	15.305	1.00	17.16	A	O
ATOM	1112	N	ASN	A	151	0.916	1.407	14.526	1.00	19.09	A	N
ATOM	1113	CA	ASN	A	151	1.834	0.850	13.538	1.00	19.75	A	C
ATOM	1114	CB	ASN	A	151	1.225	0.950	12.130	1.00	20.10	A	C
ATOM	1115	CG	ASN	A	151	-0.141	0.299	12.025	1.00	19.86	A	C
ATOM	1116	OD1	ASN	A	151	-0.239	-0.905	11.855	1.00	19.33	A	O
ATOM	1117	ND2	ASN	A	151	-1.198	1.090	12.167	1.00	19.31	A	N
ATOM	1118	C	ASN	A	151	3.150	1.599	13.557	1.00	20.21	A	C
ATOM	1119	O	ASN	A	151	3.193	2.807	13.793	1.00	22.14	A	O
ATOM	1120	N	ASP	A	152	4.239	0.911	13.299	1.00	20.04	A	N
ATOM	1121	CA	ASP	A	152	5.508	1.595	13.319	1.00	20.51	A	C
ATOM	1122	CB	BASP	A	152	6.571	0.640	13.830	0.35	20.16	A	C
ATOM	1123	CB	AASP	A	152	6.645	0.666	13.762	0.65	21.56	A	C
ATOM	1124	CG	BASP	A	152	6.199	0.067	15.205	0.35	19.09	A	C
ATOM	1125	CG	AASP	A	152	7.225	-0.117	12.631	0.65	23.76	A	C
ATOM	1126	OD1BASP	A	152	5.318	0.654	15.901	0.35	15.06	A	O	
ATOM	1127	OD1AASP	A	152	6.404	-0.719	11.924	0.65	27.77	A	O	
ATOM	1128	OD2BASP	A	152	6.703	-0.977	15.653	0.35	16.81	A	O	



ATOM	1129	OD2AASP	A	152	8.471	-0.170	12.353	0.65	27.40	A	O	
ATOM	1130	C	ASP	A	152	5.822	2.270	11.959	1.00	19.32	A	C
ATOM	1131	O	ASP	A	152	6.748	1.916	11.253	1.00	20.60	A	O
ATOM	1132	N	MET	A	153	4.988	3.250	11.628	1.00	16.58	A	N
ATOM	1133	CA	MET	A	153	5.154	4.050	10.437	1.00	16.03	A	C
ATOM	1134	CB	MET	A	153	3.876	4.007	9.619	1.00	16.23	A	C
ATOM	1135	CG	MET	A	153	3.885	4.921	8.432	1.00	18.33	A	C
ATOM	1136	SD	MET	A	153	4.694	4.182	7.030	1.00	21.72	A	S
ATOM	1137	CE	MET	A	153	3.290	3.549	6.297	1.00	21.74	A	C
ATOM	1138	C	MET	A	153	5.443	5.482	10.871	1.00	14.80	A	C
ATOM	1139	O	MET	A	153	4.684	6.058	11.646	1.00	13.50	A	O
ATOM	1140	N	THR	A	154	6.525	6.059	10.368	1.00	13.34	A	N
ATOM	1141	CA	THR	A	154	6.813	7.482	10.638	1.00	13.08	A	C
ATOM	1142	CB	THR	A	154	8.324	7.699	10.652	1.00	13.02	A	C
ATOM	1143	OG1	THR	A	154	8.886	6.949	11.724	1.00	11.51	A	O
ATOM	1144	CG2	THR	A	154	8.693	9.145	10.963	1.00	14.36	A	C
ATOM	1145	C	THR	A	154	6.153	8.310	9.573	1.00	12.50	A	C
ATOM	1146	O	THR	A	154	6.396	8.108	8.371	1.00	12.64	A	O
ATOM	1147	N	ILE	A	155	5.290	9.227	9.987	1.00	12.34	A	N
ATOM	1148	CA	ILE	A	155	4.492	10.002	9.037	1.00	13.00	A	C
ATOM	1149	CB	ILE	A	155	2.983	9.799	9.346	1.00	13.05	A	C
ATOM	1150	CG1	ILE	A	155	2.637	8.307	9.279	1.00	13.73	A	C
ATOM	1151	CD1	ILE	A	155	1.121	8.017	9.274	1.00	12.93	A	C
ATOM	1152	CG2	ILE	A	155	2.121	10.578	8.371	1.00	13.58	A	C
ATOM	1153	C	ILE	A	155	4.861	11.480	9.137	1.00	13.01	A	C
ATOM	1154	O	ILE	A	155	4.894	12.038	10.233	1.00	12.79	A	O
ATOM	1155	N	LEU	A	156	5.125	12.117	8.001	1.00	12.16	A	N
ATOM	1156	CA	LEU	A	156	5.509	13.528	7.982	1.00	12.88	A	C
ATOM	1157	CB	LEU	A	156	6.903	13.692	7.354	1.00	12.18	A	C
ATOM	1158	CG	LEU	A	156	8.089	12.960	8.007	1.00	13.25	A	C
ATOM	1159	CD1	LEU	A	156	8.365	11.607	7.326	1.00	11.24	A	C
ATOM	1160	CD2	LEU	A	156	9.339	13.796	7.910	1.00	13.01	A	C
ATOM	1161	C	LEU	A	156	4.485	14.328	7.192	1.00	13.49	A	C
ATOM	1162	O	LEU	A	156	3.982	13.850	6.160	1.00	14.76	A	O
ATOM	1163	N	PHE	A	157	4.197	15.540	7.659	1.00	12.79	A	N
ATOM	1164	CA	PHE	A	157	3.282	16.451	7.003	1.00	13.07	A	C
ATOM	1165	CB	PHE	A	157	1.938	16.564	7.772	1.00	13.62	A	C
ATOM	1166	CG	PHE	A	157	0.957	15.504	7.401	1.00	13.90	A	C
ATOM	1167	CD1	PHE	A	157	0.191	15.636	6.272	1.00	11.22	A	C
ATOM	1168	CE1	PHE	A	157	-0.678	14.632	5.896	1.00	14.22	A	C
ATOM	1169	CZ	PHE	A	157	-0.743	13.441	6.630	1.00	14.61	A	C
ATOM	1170	CE2	PHE	A	157	0.013	13.296	7.743	1.00	15.64	A	C
ATOM	1171	CD2	PHE	A	157	0.891	14.312	8.122	1.00	14.56	A	C
ATOM	1172	C	PHE	A	157	3.899	17.852	6.928	1.00	13.18	A	C
ATOM	1173	O	PHE	A	157	4.527	18.318	7.867	1.00	12.04	A	O
ATOM	1174	N	ALA	A	158	3.700	18.500	5.793	1.00	13.46	A	N
ATOM	1175	CA	ALA	A	158	3.958	19.921	5.623	1.00	13.31	A	C
ATOM	1176	CB	ALA	A	158	3.509	20.334	4.235	1.00	14.02	A	C
ATOM	1177	C	ALA	A	158	3.181	20.703	6.672	1.00	13.75	A	C
ATOM	1178	O	ALA	A	158	2.031	20.380	6.965	1.00	13.75	A	O
ATOM	1179	N	ALA	A	159	3.787	21.752	7.215	1.00	13.45	A	N
ATOM	1180	CA	ALA	A	159	3.122	22.582	8.210	1.00	13.81	A	C
ATOM	1181	CB	ALA	A	159	4.151	23.495	8.944	1.00	13.64	A	C
ATOM	1182	C	ALA	A	159	2.043	23.473	7.628	1.00	14.14	A	C
ATOM	1183	O	ALA	A	159	1.175	23.924	8.364	1.00	14.00	A	O
ATOM	1184	N	GLY	A	160	2.131	23.753	6.330	1.00	15.19	A	N
ATOM	1185	CA	GLY	A	160	1.230	24.680	5.652	1.00	15.34	A	C
ATOM	1186	C	GLY	A	160	1.957	25.941	5.236	1.00	14.93	A	C



ATOM	1187	O	GLY	A	160	3.041	26.238	5.736	1.00	14.62	A	O
ATOM	1188	N	ASN	A	161	1.371	26.686	4.307	1.00	15.04	A	N
ATOM	1189	CA	ASN	A	161	1.983	27.902	3.789	1.00	15.84	A	C
ATOM	1190	CB	ASN	A	161	2.072	27.872	2.261	1.00	15.91	A	C
ATOM	1191	CG	ASN	A	161	3.048	26.851	1.712	1.00	17.40	A	C
ATOM	1192	OD1	ASN	A	161	3.001	26.550	0.490	1.00	21.70	A	O
ATOM	1193	ND2	ASN	A	161	3.888	26.267	2.569	1.00	11.15	A	N
ATOM	1194	C	ASN	A	161	1.131	29.114	4.123	1.00	16.84	A	C
ATOM	1195	O	ASN	A	161	0.956	29.965	3.286	1.00	17.07	A	O
ATOM	1196	N	GLU	A	162	0.575	29.179	5.324	1.00	18.36	A	N
ATOM	1197	CA	GLU	A	162	-0.392	30.213	5.668	1.00	18.85	A	C
ATOM	1198	CB	GLU	A	162	-1.672	29.537	6.211	1.00	19.64	A	C
ATOM	1199	CG	GLU	A	162	-2.431	28.723	5.150	1.00	22.12	A	C
ATOM	1200	CD	GLU	A	162	-1.756	27.381	4.788	1.00	26.12	A	C
ATOM	1201	OE1	GLU	A	162	-1.585	26.545	5.702	1.00	28.48	A	O
ATOM	1202	OE2	GLU	A	162	-1.405	27.149	3.590	1.00	26.75	A	O
ATOM	1203	C	GLU	A	162	0.147	31.262	6.657	1.00	19.39	A	C
ATOM	1204	O	GLU	A	162	-0.633	32.031	7.225	1.00	18.80	A	O
ATOM	1205	N	GLY	A	163	1.472	31.338	6.820	1.00	19.39	A	N
ATOM	1206	CA	GLY	A	163	2.082	32.322	7.705	1.00	20.03	A	C
ATOM	1207	C	GLY	A	163	2.224	33.699	7.048	1.00	21.41	A	C
ATOM	1208	O	GLY	A	163	1.822	33.866	5.877	1.00	20.72	A	O
ATOM	1209	N	PRO	A	164	2.835	34.671	7.737	1.00	21.93	A	N
ATOM	1210	CA	PRO	A	164	3.496	34.491	9.053	1.00	22.22	A	C
ATOM	1211	CB	PRO	A	164	4.575	35.577	9.050	1.00	22.99	A	C
ATOM	1212	CG	PRO	A	164	3.945	36.720	8.171	1.00	23.13	A	C
ATOM	1213	CD	PRO	A	164	2.976	36.047	7.209	1.00	22.03	A	C
ATOM	1214	C	PRO	A	164	2.681	34.621	10.329	1.00	22.18	A	C
ATOM	1215	O	PRO	A	164	3.289	34.603	11.414	1.00	21.36	A	O
ATOM	1216	N	GLY	A	165	1.363	34.702	10.239	1.00	21.66	A	N
ATOM	1217	CA	GLY	A	165	0.537	34.844	11.414	1.00	21.84	A	C
ATOM	1218	C	GLY	A	165	0.522	33.581	12.243	1.00	22.27	A	C
ATOM	1219	O	GLY	A	165	0.680	32.440	11.713	1.00	22.20	A	O
ATOM	1220	N	SER	A	166	0.305	33.762	13.543	1.00	22.06	A	N
ATOM	1221	CA	SER	A	166	0.290	32.645	14.470	1.00	21.96	A	C
ATOM	1222	CB	SER	A	166	0.344	33.167	15.917	1.00	23.25	A	C
ATOM	1223	OG	SER	A	166	-0.948	33.579	16.367	1.00	25.13	A	O
ATOM	1224	C	SER	A	166	-0.954	31.807	14.241	1.00	21.45	A	C
ATOM	1225	O	SER	A	166	-1.949	32.311	13.716	1.00	21.15	A	O
ATOM	1226	N	GLY	A	167	-0.879	30.515	14.574	1.00	20.07	A	N
ATOM	1227	CA	GLY	A	167	-2.032	29.639	14.548	1.00	19.63	A	C
ATOM	1228	C	GLY	A	167	-2.478	29.248	13.140	1.00	19.18	A	C
ATOM	1229	O	GLY	A	167	-3.652	29.051	12.911	1.00	18.57	A	O
ATOM	1230	N	THR	A	168	-1.541	29.140	12.200	1.00	18.31	A	N
ATOM	1231	CA	THR	A	168	-1.893	28.857	10.810	1.00	17.13	A	C
ATOM	1232	CB	THR	A	168	-1.295	29.958	9.908	1.00	17.32	A	C
ATOM	1233	OG1	THR	A	168	0.077	30.172	10.261	1.00	14.44	A	O
ATOM	1234	CG2	THR	A	168	-1.988	31.299	10.156	1.00	17.60	A	C
ATOM	1235	C	THR	A	168	-1.496	27.465	10.306	1.00	16.75	A	C
ATOM	1236	O	THR	A	168	-1.462	27.213	9.091	1.00	16.26	A	O
ATOM	1237	N	ILE	A	169	-1.265	26.540	11.234	1.00	15.95	A	N
ATOM	1238	CA	ILE	A	169	-0.863	25.191	10.871	1.00	15.48	A	C
ATOM	1239	CB	ILE	A	169	-0.454	24.378	12.127	1.00	15.09	A	C
ATOM	1240	CG1	ILE	A	169	0.626	25.109	12.942	1.00	14.88	A	C
ATOM	1241	CD1	ILE	A	169	2.021	25.201	12.267	1.00	16.38	A	C
ATOM	1242	CG2	ILE	A	169	0.021	22.988	11.720	1.00	13.45	A	C
ATOM	1243	C	ILE	A	169	-2.004	24.477	10.137	1.00	15.22	A	C
ATOM	1244	O	ILE	A	169	-3.146	24.470	10.590	1.00	14.50	A	O

ATOM	1245	N	SER	A	170	-1.681	23.857	9.018	1.00	14.94	A	N
ATOM	1246	CA	SER	A	170	-2.665	23.060	8.310	1.00	15.41	A	C
ATOM	1247	CB	SER	A	170	-2.299	23.004	6.821	1.00	16.02	A	C
ATOM	1248	OG	SER	A	170	-1.040	22.404	6.585	1.00	16.03	A	O
ATOM	1249	C	SER	A	170	-2.855	21.660	8.904	1.00	15.05	A	C
ATOM	1250	O	SER	A	170	-1.986	21.137	9.616	1.00	13.80	A	O
ATOM	1251	N	ALA	A	171	-3.992	21.036	8.582	1.00	14.65	A	N
ATOM	1252	CA	ALA	A	171	-4.244	19.651	8.933	1.00	14.75	A	C
ATOM	1253	CB	ALA	A	171	-5.700	19.507	9.443	1.00	15.62	A	C
ATOM	1254	C	ALA	A	171	-4.043	18.750	7.740	1.00	15.02	A	C
ATOM	1255	O	ALA	A	171	-4.475	19.096	6.652	1.00	14.12	A	O
ATOM	1256	N	PRO	A	172	-3.482	17.548	7.899	1.00	15.48	A	N
ATOM	1257	CA	PRO	A	172	-3.078	16.913	9.167	1.00	15.17	A	C
ATOM	1258	CB	PRO	A	172	-3.080	15.411	8.796	1.00	15.90	A	C
ATOM	1259	CG	PRO	A	172	-3.707	15.336	7.456	1.00	15.73	A	C
ATOM	1260	CD	PRO	A	172	-3.401	16.614	6.768	1.00	15.43	A	C
ATOM	1261	C	PRO	A	172	-1.724	17.260	9.788	1.00	14.85	A	C
ATOM	1262	O	PRO	A	172	-1.284	16.499	10.651	1.00	16.20	A	O
ATOM	1263	N	GLY	A	173	-1.086	18.352	9.382	1.00	14.01	A	N
ATOM	1264	CA	GLY	A	173	0.078	18.895	10.064	1.00	13.48	A	C
ATOM	1265	C	GLY	A	173	-0.158	19.147	11.553	1.00	13.91	A	C
ATOM	1266	O	GLY	A	173	0.809	19.174	12.339	1.00	14.08	A	O
ATOM	1267	N	THR	A	174	-1.419	19.291	11.956	1.00	13.50	A	N
ATOM	1268	CA	THR	A	174	-1.758	19.475	13.375	1.00	13.19	A	C
ATOM	1269	CB	THR	A	174	-3.137	20.125	13.530	1.00	13.66	A	C
ATOM	1270	OG1	THR	A	174	-4.104	19.394	12.743	1.00	13.16	A	O
ATOM	1271	CG2	THR	A	174	-3.114	21.510	12.957	1.00	14.22	A	C
ATOM	1272	C	THR	A	174	-1.774	18.188	14.172	1.00	12.85	A	C
ATOM	1273	O	THR	A	174	-1.909	18.227	15.390	1.00	12.08	A	O
ATOM	1274	N	ALA	A	175	-1.696	17.040	13.505	1.00	12.94	A	N
ATOM	1275	CA	ALA	A	175	-1.614	15.772	14.213	1.00	12.90	A	C
ATOM	1276	CB	ALA	A	175	-1.422	14.641	13.211	1.00	13.54	A	C
ATOM	1277	C	ALA	A	175	-0.484	15.740	-15.264	1.00	12.44	A	C
ATOM	1278	O	ALA	A	175	0.601	16.233	15.043	1.00	13.06	A	O
ATOM	1279	N	LYS	A	176	-0.739	15.131	16.398	1.00	13.08	A	N
ATOM	1280	CA	LYS	A	176	0.269	15.057	17.466	1.00	13.00	A	C
ATOM	1281	CB	LYS	A	176	-0.383	14.511	18.719	1.00	12.78	A	C
ATOM	1282	CG	LYS	A	176	-1.406	15.392	19.366	1.00	13.87	A	C
ATOM	1283	CD	LYS	A	176	-2.044	14.693	20.553	1.00	15.77	A	C
ATOM	1284	CE	LYS	A	176	-3.179	13.722	20.173	1.00	16.63	A	C
ATOM	1285	NZ	LYS	A	176	-3.738	13.048	21.388	1.00	16.58	A	N
ATOM	1286	C	LYS	A	176	1.433	14.107	17.115	1.00	13.10	A	C
ATOM	1287	O	LYS	A	176	2.559	14.289	17.538	1.00	12.98	A	O
ATOM	1288	N	ASN	A	177	1.119	13.047	16.390	1.00	12.81	A	N
ATOM	1289	CA	ASN	A	177	2.047	11.933	16.187	1.00	12.78	A	C
ATOM	1290	CB	ASN	A	177	1.278	10.628	16.301	1.00	12.48	A	C
ATOM	1291	CG	ASN	A	177	0.733	10.382	17.718	1.00	12.12	A	C
ATOM	1292	OD1	ASN	A	177	1.135	11.043	18.682	1.00	12.31	A	O
ATOM	1293	ND2	ASN	A	177	-0.179	9.416	17.844	1.00	10.81	A	N
ATOM	1294	C	ASN	A	177	2.822	11.966	14.876	1.00	12.68	A	C
ATOM	1295	O	ASN	A	177	3.692	11.097	14.621	1.00	13.33	A	O
ATOM	1296	N	ALA	A	178	2.483	12.933	14.029	1.00	12.80	A	N
ATOM	1297	CA	ALA	A	178	3.234	13.208	12.801	1.00	12.70	A	C
ATOM	1298	CB	ALA	A	178	2.382	13.938	11.817	1.00	12.83	A	C
ATOM	1299	C	ALA	A	178	4.439	14.052	13.141	1.00	12.18	A	C
ATOM	1300	O	ALA	A	178	4.471	14.685	14.188	1.00	12.29	A	O
ATOM	1301	N	ILE	A	179	5.458	13.985	12.293	1.00	11.71	A	N
ATOM	1302	CA	ILE	A	179	6.531	14.966	12.283	1.00	11.72	A	C

ATOM	1303	CB	ILE	A	179	7.838	14.364	11.812	1.00	11.54	A	C
ATOM	1304	CG1	ILE	A	179	8.251	13.222	12.712	1.00	13.45	A	C
ATOM	1305	CD1	ILE	A	179	9.472	12.467	12.196	1.00	14.82	A	C
ATOM	1306	CG2	ILE	A	179	8.927	15.437	11.783	1.00	12.00	A	C
ATOM	1307	C	ILE	A	179	6.085	16.076	11.317	1.00	11.98	A	C
ATOM	1308	O	ILE	A	179	5.943	15.852	10.109	1.00	11.31	A	O
ATOM	1309	N	THR	A	180	5.813	17.248	11.871	1.00	11.27	A	N
ATOM	1310	CA	THR	A	180	5.357	18.383	11.074	1.00	11.76	A	C
ATOM	1311	CB	THR	A	180	4.260	19.120	11.818	1.00	11.79	A	C
ATOM	1312	OG1	THR	A	180	3.166	18.214	12.084	1.00	12.06	A	O
ATOM	1313	CG2	THR	A	180	3.603	20.224	10.929	1.00	12.72	A	C
ATOM	1314	C	THR	A	180	6.530	19.306	10.690	1.00	11.82	A	C
ATOM	1315	O	THR	A	180	7.286	19.762	11.533	1.00	11.02	A	O
ATOM	1316	N	VAL	A	181	6.662	19.590	9.401	1.00	11.42	A	N
ATOM	1317	CA	VAL	A	181	7.830	20.305	8.899	1.00	11.43	A	C
ATOM	1318	CB	VAL	A	181	8.492	19.464	7.814	1.00	11.32	A	C
ATOM	1319	CG1	VAL	A	181	9.744	20.118	7.309	1.00	12.42	A	C
ATOM	1320	CG2	VAL	A	181	8.757	18.055	8.351	1.00	12.33	A	C
ATOM	1321	C	VAL	A	181	7.511	21.680	8.302	1.00	11.62	A	C
ATOM	1322	O	VAL	A	181	6.667	21.800	7.399	1.00	12.16	A	O
ATOM	1323	N	GLY	A	182	8.187	22.704	8.812	1.00	11.59	A	N
ATOM	1324	CA	GLY	A	182	8.095	24.042	8.273	1.00	12.80	A	C
ATOM	1325	C	GLY	A	182	9.296	24.352	7.391	1.00	13.72	A	C
ATOM	1326	O	GLY	A	182	10.243	23.574	7.344	1.00	14.13	A	O
ATOM	1327	N	ALA	A	183	9.264	25.492	6.700	1.00	13.43	A	N
ATOM	1328	CA	ALA	A	183	10.312	25.837	5.776	1.00	14.22	A	C
ATOM	1329	CB	ALA	A	183	9.709	26.166	4.401	1.00	14.53	A	C
ATOM	1330	C	ALA	A	183	11.205	27.001	6.238	1.00	14.32	A	C
ATOM	1331	O	ALA	A	183	10.717	28.110	6.498	1.00	14.13	A	O
ATOM	1332	N	THR	A	184	12.512	26.737	6.293	1.00	14.17	A	N
ATOM	1333	CA	THR	A	184	13.513	27.799	6.294	1.00	14.33	A	C
ATOM	1334	CB	THR	A	184	14.743	27.451	7.159	1.00	14.19	A	C
ATOM	1335	OG1	THR	A	184	15.180	26.103	6.925	1.00	13.83	A	O
ATOM	1336	CG2	THR	A	184	14.383	27.474	8.636	1.00	13.70	A	C
ATOM	1337	C	THR	A	184	13.905	28.018	4.841	1.00	15.47	A	C
ATOM	1338	O	THR	A	184	13.380	27.354	3.934	1.00	15.87	A	O
ATOM	1339	N	GLU	A	185	14.861	28.919	4.618	1.00	15.13	A	N
ATOM	1340	CA	GLU	A	185	15.328	29.246	3.290	1.00	14.03	A	C
ATOM	1341	CB	GLU	A	185	15.696	30.766	3.230	1.00	13.82	A	C
ATOM	1342	CG	GLU	A	185	14.492	31.673	3.495	1.00	15.09	A	C
ATOM	1343	CD	GLU	A	185	14.785	33.172	3.329	1.00	14.09	A	C
ATOM	1344	OE1	GLU	A	185	15.911	33.541	2.985	1.00	15.60	A	O
ATOM	1345	OE2	GLU	A	185	13.871	33.984	3.528	1.00	14.21	A	O
ATOM	1346	C	GLU	A	185	16.511	28.376	2.863	1.00	13.70	A	C
ATOM	1347	O	GLU	A	185	17.387	28.011	3.675	1.00	14.17	A	O
ATOM	1348	N	ASN	A	186	16.521	28.008	1.587	1.00	12.64	A	N
ATOM	1349	CA	ASN	A	186	17.707	27.452	0.959	1.00	13.44	A	C
ATOM	1350	CB	ASN	A	186	17.345	26.758	-0.353	1.00	13.84	A	C
ATOM	1351	CG	ASN	A	186	18.293	25.630	-0.717	1.00	14.82	A	C
ATOM	1352	OD1	ASN	A	186	19.084	25.169	0.099	1.00	14.62	A	O
ATOM	1353	ND2	ASN	A	186	18.189	25.156	-1.970	1.00	15.51	A	N
ATOM	1354	C	ASN	A	186	18.652	28.603	0.681	1.00	13.83	A	C
ATOM	1355	O	ASN	A	186	18.244	29.769	0.711	1.00	14.50	A	O
ATOM	1356	N	LEU	A	187	19.920	28.298	0.470	1.00	14.83	A	N
ATOM	1357	CA	LEU	A	187	20.892	29.352	0.213	1.00	14.62	A	C
ATOM	1358	CB	LEU	A	187	22.144	29.144	1.018	1.00	15.48	A	C
ATOM	1359	CG	LEU	A	187	23.144	30.319	0.975	1.00	17.25	A	C
ATOM	1360	CD1	LEU	A	187	22.504	31.587	1.469	1.00	18.56	A	C

ATOM	1361	CD2	LEU	A	187	24.394	29.973	1.816	1.00	20.46	A	C
ATOM	1362	C	LEU	A	187	21.205	29.360	-1.279	1.00	14.80	A	C
ATOM	1363	O	LEU	A	187	22.106	28.692	-1.734	1.00	14.07	A	O
ATOM	1364	N	ARG	A	188	20.398	30.083	-2.023	1.00	15.63	A	N
ATOM	1365	CA	ARG	A	188	20.631	30.308	-3.454	1.00	17.55	A	C
ATOM	1366	CB	ARG	A	188	19.658	29.484	-4.273	1.00	17.02	A	C
ATOM	1367	CG	ARG	A	188	19.842	27.989	-4.168	1.00	17.82	A	C
ATOM	1368	CD	ARG	A	188	19.063	27.213	-5.267	1.00	19.96	A	C
ATOM	1369	NE	ARG	A	188	19.315	25.782	-5.224	1.00	18.26	A	N
ATOM	1370	CZ	ARG	A	188	20.339	25.172	-5.814	1.00	19.52	A	C
ATOM	1371	NH1	ARG	A	188	21.235	25.846	-6.530	1.00	17.91	A	N
ATOM	1372	NH2	ARG	A	188	20.475	23.867	-5.693	1.00	19.41	A	N
ATOM	1373	C	ARG	A	188	20.387	31.804	-3.694	1.00	17.89	A	C
ATOM	1374	O	ARG	A	188	19.379	32.189	-4.251	1.00	18.33	A	O
ATOM	1375	N	PRO	A	189	21.273	32.646	-3.181	1.00	19.58	A	N
ATOM	1376	CA	PRO	A	189	20.990	34.082	-3.061	1.00	20.68	A	C
ATOM	1377	CB	PRO	A	189	22.179	34.613	-2.239	1.00	21.07	A	C
ATOM	1378	CG	PRO	A	189	23.271	33.608	-2.417	1.00	21.15	A	C
ATOM	1379	CD	PRO	A	189	22.599	32.288	-2.657	1.00	20.12	A	C
ATOM	1380	C	PRO	A	189	20.833	34.863	-4.373	1.00	21.39	A	C
ATOM	1381	O	PRO	A	189	20.276	35.975	-4.347	1.00	20.51	A	O
ATOM	1382	N	SER	A	190	21.285	34.307	-5.492	1.00	22.89	A	N
ATOM	1383	CA	SER	A	190	21.033	34.940	-6.796	1.00	24.65	A	C
ATOM	1384	CB	SER	A	190	21.685	34.135	-7.932	1.00	24.76	A	C
ATOM	1385	OG	SER	A	190	21.082	32.831	-8.046	1.00	25.85	A	O
ATOM	1386	C	SER	A	190	19.525	35.098	-7.028	1.00	25.23	A	C
ATOM	1387	O	SER	A	190	19.080	35.918	-7.850	1.00	26.47	A	O
ATOM	1388	N	PHE	A	191	18.723	34.365	-6.258	1.00	25.36	A	N
ATOM	1389	CA	PHE	A	191	17.264	34.446	-6.389	1.00	25.28	A	C
ATOM	1390	CB	PHE	A	191	16.643	33.046	-6.156	1.00	25.00	A	C
ATOM	1391	CG	PHE	A	191	16.841	32.089	-7.310	1.00	23.34	A	C
ATOM	1392	CD1	PHE	A	191	17.565	30.932	-7.159	1.00	21.81	A	C
ATOM	1393	CE1	PHE	A	191	17.735	30.052	-8.218	1.00	22.63	A	C
ATOM	1394	CZ	PHE	A	191	17.180	30.341	-9.470	1.00	21.46	A	C
ATOM	1395	CE2	PHE	A	191	16.449	31.484	-9.631	1.00	22.61	A	C
ATOM	1396	CD2	PHE	A	191	16.288	32.361	-8.562	1.00	25.47	A	C
ATOM	1397	C	PHE	A	191	16.388	35.561	-5.720	1.00	25.71	A	C
ATOM	1398	O	PHE	A	191	15.184	35.500	-5.877	1.00	27.33	A	O
ATOM	1399	N	GLY	A	192	16.823	36.552	-4.944	1.00	26.98	A	N
ATOM	1400	CA	GLY	A	192	17.639	36.484	-3.783	1.00	26.29	A	C
ATOM	1401	C	GLY	A	192	16.795	36.445	-2.478	1.00	25.37	A	C
ATOM	1402	O	GLY	A	192	17.008	35.528	-1.733	1.00	25.24	A	O
ATOM	1403	N	SER	A	193	15.858	37.355	-2.179	1.00	24.49	A	N
ATOM	1404	CA	SER	A	193	15.332	37.444	-0.778	1.00	24.39	A	C
ATOM	1405	CB	SER	A	193	14.452	38.689	-0.554	1.00	24.51	A	C
ATOM	1406	OG	SER	A	193	13.058	38.407	-0.623	1.00	25.19	A	O
ATOM	1407	C	SER	A	193	14.664	36.176	-0.133	1.00	23.94	A	C
ATOM	1408	O	SER	A	193	14.740	35.973	1.085	1.00	22.27	A	O
ATOM	1409	N	TYR	A	194	14.037	35.331	-0.949	1.00	23.39	A	N
ATOM	1410	CA	TYR	A	194	13.497	34.046	-0.477	1.00	23.08	A	C
ATOM	1411	CB	TYR	A	194	12.407	33.559	-1.439	1.00	23.87	A	C
ATOM	1412	CG	TYR	A	194	11.044	34.129	-1.144	1.00	27.80	A	C
ATOM	1413	CD1	TYR	A	194	10.563	35.240	-1.832	1.00	31.12	A	C
ATOM	1414	CE1	TYR	A	194	9.317	35.775	-1.554	1.00	32.91	A	C
ATOM	1415	CZ	TYR	A	194	8.525	35.182	-0.591	1.00	34.12	A	C
ATOM	1416	OH	TYR	A	194	7.282	35.696	-0.311	1.00	38.22	A	O
ATOM	1417	CE2	TYR	A	194	8.974	34.076	0.108	1.00	33.28	A	C
ATOM	1418	CD2	TYR	A	194	10.229	33.556	-0.169	1.00	31.26	A	C



ATOM	1419	C	TYR	A	194	14.545	32.930	-0.289	1.00	21.59	A	C
ATOM	1420	O	TYR	A	194	14.225	31.848	0.236	1.00	20.33	A	O
ATOM	1421	N	ALA	A	195	15.785	33.185	-0.695	1.00	20.44	A	N
ATOM	1422	CA	ALA	A	195	16.838	32.181	-0.610	1.00	20.47	A	C
ATOM	1423	CB	ALA	A	195	16.915	31.365	-1.892	1.00	20.41	A	C
ATOM	1424	C	ALA	A	195	18.222	32.757	-0.270	1.00	19.93	A	C
ATOM	1425	O	ALA	A	195	19.230	32.354	-0.877	1.00	19.21	A	O
ATOM	1426	N	ASP	A	196	18.264	33.615	0.750	1.00	19.15	A	N
ATOM	1427	CA	ASP	A	196	19.472	34.355	1.126	1.00	19.86	A	C
ATOM	1428	CB	ASP	A	196	19.264	35.861	0.919	1.00	20.04	A	C
ATOM	1429	CG	ASP	A	196	18.198	36.453	1.814	1.00	22.11	A	C
ATOM	1430	OD1	ASP	A	196	18.040	37.693	1.696	1.00	23.87	A	O
ATOM	1431	OD2	ASP	A	196	17.461	35.822	2.649	1.00	19.55	A	O
ATOM	1432	C	ASP	A	196	20.025	34.163	2.549	1.00	19.90	A	C
ATOM	1433	O	ASP	A	196	21.092	34.705	2.869	1.00	19.61	A	O
ATOM	1434	N	ASN	A	197	19.326	33.410	3.394	1.00	18.85	A	N
ATOM	1435	CA	ASN	A	197	19.790	33.177	4.757	1.00	18.29	A	C
ATOM	1436	CB	ASN	A	197	19.410	34.369	5.644	1.00	18.68	A	C
ATOM	1437	CG	ASN	A	197	20.123	34.360	7.001	1.00	19.48	A	C
ATOM	1438	OD1	ASN	A	197	20.221	33.319	7.630	1.00	16.60	A	O
ATOM	1439	ND2	ASN	A	197	20.603	35.541	7.455	1.00	14.55	A	N
ATOM	1440	C	ASN	A	197	19.198	31.861	5.304	1.00	17.30	A	C
ATOM	1441	O	ASN	A	197	17.986	31.734	5.463	1.00	16.96	A	O
ATOM	1442	N	ILE	A	198	20.066	30.901	5.608	1.00	16.67	A	N
ATOM	1443	CA	ILE	A	198	19.606	29.557	5.993	1.00	16.04	A	C
ATOM	1444	CB	ILE	A	198	20.771	28.571	6.020	1.00	15.64	A	C
ATOM	1445	CG1	ILE	A	198	21.724	28.885	7.179	1.00	16.27	A	C
ATOM	1446	CD1	ILE	A	198	22.734	27.781	7.490	1.00	18.08	A	C
ATOM	1447	CG2	ILE	A	198	21.459	28.530	4.679	1.00	16.50	A	C
ATOM	1448	C	ILE	A	198	18.897	29.560	7.352	1.00	15.03	A	C
ATOM	1449	O	ILE	A	198	18.222	28.605	7.723	1.00	15.12	A	O
ATOM	1450	N	ASN	A	199	19.054	30.642	8.102	1.00	14.78	A	N
ATOM	1451	CA	ASN	A	199	18.316	30.794	9.344	1.00	14.68	A	C
ATOM	1452	CB	ASN	A	199	19.180	31.609	10.332	1.00	14.98	A	C
ATOM	1453	CG	ASN	A	199	20.487	30.948	10.708	1.00	15.69	A	C
ATOM	1454	OD1	ASN	A	199	20.560	29.757	10.907	1.00	14.98	A	O
ATOM	1455	ND2	ASN	A	199	21.526	31.768	10.903	1.00	20.04	A	N
ATOM	1456	C	ASN	A	199	17.036	31.597	9.311	1.00	14.49	A	C
ATOM	1457	O	ASN	A	199	16.239	31.490	10.227	1.00	14.69	A	O
ATOM	1458	N	HIS	A	200	16.736	32.328	8.241	1.00	15.73	A	N
ATOM	1459	CA	HIS	A	200	15.375	32.648	7.854	1.00	14.99	A	C
ATOM	1460	CB	HIS	A	200	15.338	33.612	6.641	1.00	15.17	A	C
ATOM	1461	CG	HIS	A	200	16.005	34.942	6.871	1.00	17.24	A	C
ATOM	1462	ND1	HIS	A	200	16.242	35.840	5.842	1.00	16.94	A	N
ATOM	1463	CE1	HIS	A	200	16.842	36.916	6.327	1.00	19.73	A	C
ATOM	1464	NE2	HIS	A	200	17.009	36.751	7.628	1.00	17.79	A	N
ATOM	1465	CD2	HIS	A	200	16.469	35.538	7.999	1.00	18.37	A	C
ATOM	1466	C	HIS	A	200	14.327	31.581	7.730	1.00	15.01	A	C
ATOM	1467	O	HIS	A	200	14.472	30.673	6.965	1.00	14.41	A	O
ATOM	1468	N	VAL	A	201	13.251	31.772	8.496	1.00	15.72	A	N
ATOM	1469	CA	VAL	A	201	12.004	31.059	8.294	1.00	16.37	A	C
ATOM	1470	CB	VAL	A	201	11.103	31.185	9.523	1.00	16.41	A	C
ATOM	1471	CG1	VAL	A	201	9.780	30.428	9.297	1.00	16.12	A	C
ATOM	1472	CG2	VAL	A	201	11.841	30.668	10.783	1.00	18.01	A	C
ATOM	1473	C	VAL	A	201	11.313	31.683	7.089	1.00	16.94	A	C
ATOM	1474	O	VAL	A	201	11.250	32.900	6.973	1.00	17.09	A	O
ATOM	1475	N	ALA	A	202	10.872	30.865	6.143	1.00	17.70	A	N
ATOM	1476	CA	ALA	A	202	10.233	31.396	4.949	1.00	17.52	A	C



ATOM	1477	CB	ALA	A	202	9.859	30.265	4.018	1.00	18.76	A	C
ATOM	1478	C	ALA	A	202	9.000	32.169	5.383	1.00	17.84	A	C
ATOM	1479	O	ALA	A	202	8.263	31.734	6.263	1.00	16.60	A	O
ATOM	1480	N	GLN	A	203	8.770	33.332	4.783	1.00	18.20	A	N
ATOM	1481	CA	GLN	A	203	7.629	34.135	5.192	1.00	19.45	A	C
ATOM	1482	CB	BGLN	A	203	7.542	35.347	4.260	0.40	19.94	A	C
ATOM	1483	CB	AGLN	A	203	7.529	35.467	4.445	0.60	20.39	A	C
ATOM	1484	CG	BGLN	A	203	7.527	36.681	4.943	0.40	22.36	A	C
ATOM	1485	CG	AGLN	A	203	6.748	36.514	5.261	0.60	24.58	A	C
ATOM	1486	CD	BGLN	A	203	6.379	37.556	4.452	0.40	25.52	A	C
ATOM	1487	CD	AGLN	A	203	7.553	37.090	6.439	0.60	28.39	A	C
ATOM	1488	OE1BGLN	A	203	5.568	37.122	3.624	0.40	27.97	A	O	
ATOM	1489	OE1AGLN	A	203	8.525	37.816	6.236	0.60	33.69	A	O	
ATOM	1490	NE2BGLN	A	203	6.299	38.772	4.972	0.40	24.61	A	N	
ATOM	1491	NE2AGLN	A	203	7.155	36.751	7.655	0.60	31.16	A	N	
ATOM	1492	C	GLN	A	203	6.291	33.391	5.152	1.00	18.58	A	C
ATOM	1493	O	GLN	A	203	5.458	33.580	6.028	1.00	18.67	A	O
ATOM	1494	N	PHE	A	204	6.090	32.533	4.163	1.00	17.22	A	N
ATOM	1495	CA	PHE	A	204	4.805	31.833	4.027	1.00	16.75	A	C
ATOM	1496	CB	PHE	A	204	4.603	31.335	2.589	1.00	16.25	A	C
ATOM	1497	CG	PHE	A	204	5.720	30.475	2.093	1.00	16.52	A	C
ATOM	1498	CD1	PHE	A	204	5.857	29.158	2.526	1.00	16.66	A	C
ATOM	1499	CE1	PHE	A	204	6.893	28.378	2.083	1.00	17.13	A	C
ATOM	1500	CZ	PHE	A	204	7.854	28.909	1.234	1.00	14.67	A	C
ATOM	1501	CE2	PHE	A	204	7.747	30.231	0.816	1.00	16.10	A	C
ATOM	1502	CD2	PHE	A	204	6.693	31.009	1.267	1.00	15.39	A	C
ATOM	1503	C	PHE	A	204	4.670	30.647	5.018	1.00	16.21	A	C
ATOM	1504	O	PHE	A	204	3.570	30.150	5.198	1.00	15.42	A	O
ATOM	1505	N	SER	A	205	5.754	30.223	5.688	1.00	15.36	A	N
ATOM	1506	CA	SER	A	205	5.692	28.983	6.508	1.00	15.18	A	C
ATOM	1507	CB	SER	A	205	7.068	28.579	7.063	1.00	15.27	A	C
ATOM	1508	OG	SER	A	205	7.042	27.254	7.585	1.00	15.10	A	O
ATOM	1509	C	SER	A	205	4.657	29.103	7.615	1.00	14.84	A	C
ATOM	1510	O	SER	A	205	4.618	30.092	8.319	1.00	16.26	A	O
ATOM	1511	N	SER	A	206	3.764	28.141	7.753	1.00	15.82	A	N
ATOM	1512	CA	SER	A	206	2.751	28.237	8.818	1.00	15.73	A	C
ATOM	1513	CB	SER	A	206	1.714	27.117	8.735	1.00	16.10	A	C
ATOM	1514	OG	SER	A	206	0.811	27.350	7.655	1.00	14.83	A	O
ATOM	1515	C	SER	A	206	3.421	28.221	10.186	1.00	15.92	A	C
ATOM	1516	O	SER	A	206	4.486	27.589	10.362	1.00	15.30	A	O
ATOM	1517	N	ARG	A	207	2.786	28.928	11.113	1.00	15.72	A	N
ATOM	1518	CA	ARG	A	207	3.289	29.140	12.455	1.00	16.34	A	C
ATOM	1519	CB	ARG	A	207	3.511	30.636	12.715	1.00	16.50	A	C
ATOM	1520	CG	ARG	A	207	4.189	31.375	11.542	1.00	18.52	A	C
ATOM	1521	CD	ARG	A	207	5.604	30.916	11.227	1.00	20.29	A	C
ATOM	1522	NE	ARG	A	207	6.146	31.519	10.012	1.00	22.13	A	N
ATOM	1523	CZ	ARG	A	207	6.821	32.643	9.981	1.00	22.20	A	C
ATOM	1524	NH1	ARG	A	207	7.056	33.294	11.080	1.00	25.41	A	N
ATOM	1525	NH2	ARG	A	207	7.256	33.124	8.838	1.00	24.08	A	N
ATOM	1526	C	ARG	A	207	2.330	28.556	13.471	1.00	15.97	A	C
ATOM	1527	O	ARG	A	207	1.096	28.605	13.301	1.00	15.01	A	O
ATOM	1528	N	GLY	A	208	2.903	27.974	14.521	1.00	15.16	A	N
ATOM	1529	CA	GLY	A	208	2.139	27.523	15.655	1.00	16.14	A	C
ATOM	1530	C	GLY	A	208	1.622	28.688	16.476	1.00	16.50	A	C
ATOM	1531	O	GLY	A	208	1.753	29.830	16.059	1.00	17.36	A	O
ATOM	1532	N	PRO	A	209	0.999	28.423	17.617	1.00	17.42	A	N
ATOM	1533	CA	PRO	A	209	0.727	27.067	18.089	1.00	17.56	A	C
ATOM	1534	CB	PRO	A	209	0.407	27.269	19.579	1.00	17.58	A	C

ATOM	1535	CG	PRO	A	209	-0.088	28.644	19.701	1.00	18.85	A	C
ATOM	1536	CD	PRO	A	209	0.477	29.457	18.545	1.00	17.85	A	C
ATOM	1537	C	PRO	A	209	-0.483	26.483	17.368	1.00	17.50	A	C
ATOM	1538	O	PRO	A	209	-1.094	27.157	16.558	1.00	18.18	A	O
ATOM	1539	N	THR	A	210	-0.816	25.240	17.652	1.00	16.70	A	N
ATOM	1540	CA	THR	A	210	-2.050	24.690	17.186	1.00	17.34	A	C
ATOM	1541	CB	THR	A	210	-2.042	23.181	17.356	1.00	16.73	A	C
ATOM	1542	OG1	THR	A	210	-1.848	22.859	18.734	1.00	18.34	A	O
ATOM	1543	CG2	THR	A	210	-0.833	22.540	16.574	1.00	16.90	A	C
ATOM	1544	C	THR	A	210	-3.206	25.327	17.987	1.00	17.55	A	C
ATOM	1545	O	THR	A	210	-2.990	26.095	18.930	1.00	16.40	A	O
ATOM	1546	N	ARG	A	211	-4.421	24.979	17.623	1.00	18.89	A	N
ATOM	1547	CA	ARG	A	211	-5.595	25.577	18.264	1.00	20.56	A	C
ATOM	1548	CB	ARG	A	211	-6.884	25.056	17.638	1.00	21.16	A	C
ATOM	1549	CG	ARG	A	211	-8.149	25.719	18.255	1.00	25.92	A	C
ATOM	1550	CD	ARG	A	211	-9.325	25.804	17.301	1.00	31.08	A	C
ATOM	1551	NE	ARG	A	211	-8.956	26.457	16.042	1.00	35.63	A	N
ATOM	1552	CZ	ARG	A	211	-9.626	26.296	14.905	1.00	38.91	A	C
ATOM	1553	NH1	ARG	A	211	-10.707	25.516	14.876	1.00	40.64	A	N
ATOM	1554	NH2	ARG	A	211	-9.225	26.911	13.795	1.00	37.74	A	N
ATOM	1555	C	ARG	A	211	-5.591	25.308	19.768	1.00	20.16	A	C
ATOM	1556	O	ARG	A	211	-5.983	26.180	20.539	1.00	19.93	A	O
ATOM	1557	N	ASP	A	212	-5.120	24.121	20.185	1.00	19.40	A	N
ATOM	1558	CA	ASP	A	212	-5.031	23.791	21.616	1.00	18.64	A	C
ATOM	1559	CB	ASP	A	212	-5.346	22.306	21.877	1.00	18.58	A	C
ATOM	1560	CG	ASP	A	212	-4.318	21.356	21.254	1.00	16.59	A	C
ATOM	1561	OD1	ASP	A	212	-4.255	20.180	21.679	1.00	16.40	A	O
ATOM	1562	OD2	ASP	A	212	-3.545	21.688	20.339	1.00	17.56	A	O
ATOM	1563	C	ASP	A	212	-3.693	24.160	22.255	1.00	18.83	A	C
ATOM	1564	O	ASP	A	212	-3.387	23.707	23.370	1.00	19.22	A	O
ATOM	1565	N	GLY	A	213	-2.902	24.966	21.556	1.00	18.29	A	N
ATOM	1566	CA	GLY	A	213	-1.698	25.572	22.111	1.00	18.10	A	C
ATOM	1567	C	GLY	A	213	-0.439	24.713	22.065	1.00	17.75	A	C
ATOM	1568	O	GLY	A	213	0.517	24.998	22.785	1.00	18.06	A	O
ATOM	1569	N	ARG	A	214	-0.431	23.665	21.242	1.00	16.43	A	N
ATOM	1570	CA	ARG	A	214	0.757	22.826	21.110	1.00	16.72	A	C
ATOM	1571	CB	ARG	A	214	0.403	21.461	20.536	1.00	16.17	A	C
ATOM	1572	CG	ARG	A	214	-0.276	20.553	21.473	1.00	16.40	A	C
ATOM	1573	CD	ARG	A	214	-0.753	19.301	20.814	1.00	16.61	A	C
ATOM	1574	NE	ARG	A	214	-1.771	19.613	19.826	1.00	16.67	A	N
ATOM	1575	CZ	ARG	A	214	-1.740	19.297	18.531	1.00	16.71	A	C
ATOM	1576	NH1	ARG	A	214	-0.720	18.628	17.981	1.00	16.55	A	N
ATOM	1577	NH2	ARG	A	214	-2.762	19.664	17.776	1.00	14.42	A	N
ATOM	1578	C	ARG	A	214	1.772	23.493	20.203	1.00	16.16	A	C
ATOM	1579	O	ARG	A	214	1.403	24.306	19.344	1.00	16.86	A	O
ATOM	1580	N	ILE	A	215	3.046	23.168	20.396	1.00	15.82	A	N
ATOM	1581	CA	ILE	A	215	4.107	23.640	19.516	1.00	15.40	A	C
ATOM	1582	CB	ILE	A	215	5.503	23.498	20.175	1.00	16.18	A	C
ATOM	1583	CG1	ILE	A	215	5.600	24.351	21.454	1.00	17.35	A	C
ATOM	1584	CD1	ILE	A	215	5.526	25.842	21.181	1.00	20.01	A	C
ATOM	1585	CG2	ILE	A	215	6.606	23.898	19.191	1.00	15.87	A	C
ATOM	1586	C	ILE	A	215	4.100	22.834	18.214	1.00	15.40	A	C
ATOM	1587	O	ILE	A	215	4.316	21.616	18.227	1.00	14.96	A	O
ATOM	1588	N	LYS	A	216	3.841	23.536	17.117	1.00	14.61	A	N
ATOM	1589	CA	LYS	A	216	4.072	23.062	15.745	1.00	14.64	A	C
ATOM	1590	CB	LYS	A	216	2.765	22.616	15.067	1.00	13.98	A	C
ATOM	1591	CG	LYS	A	216	2.190	21.271	15.526	1.00	13.46	A	C
ATOM	1592	CD	LYS	A	216	3.073	20.102	15.117	1.00	14.36	A	C

ATOM	1593	CE	LYS	A	216	2.427	18.754	15.453	1.00	13.24	A	C
ATOM	1594	NZ	LYS	A	216	3.042	17.577	14.739	1.00	8.08	A	N
ATOM	1595	C	LYS	A	216	4.632	24.269	14.984	1.00	14.70	A	C
ATOM	1596	O	LYS	A	216	4.336	25.428	15.358	1.00	13.92	A	O
ATOM	1597	N	PRO	A	217	5.410	24.032	13.921	1.00	14.59	A	N
ATOM	1598	CA	PRO	A	217	5.788	22.691	13.468	1.00	13.65	A	C
ATOM	1599	CB	PRO	A	217	6.452	22.944	12.115	1.00	14.58	A	C
ATOM	1600	CG	PRO	A	217	6.934	24.356	12.178	1.00	15.23	A	C
ATOM	1601	CD	PRO	A	217	6.012	25.077	13.086	1.00	14.44	A	C
ATOM	1602	C	PRO	A	217	6.818	22.089	14.401	1.00	12.99	A	C
ATOM	1603	O	PRO	A	217	7.262	22.738	15.379	1.00	12.11	A	O
ATOM	1604	N	ASP	A	218	7.201	20.847	14.126	1.00	11.74	A	N
ATOM	1605	CA	ASP	A	218	8.188	20.214	14.974	1.00	11.35	A	C
ATOM	1606	CB	ASP	A	218	8.033	18.694	14.962	1.00	11.47	A	C
ATOM	1607	CG	ASP	A	218	6.672	18.241	15.451	1.00	11.82	A	C
ATOM	1608	OD1	ASP	A	218	6.440	18.370	16.680	1.00	10.57	A	O
ATOM	1609	OD2	ASP	A	218	5.810	17.726	14.671	1.00	11.50	A	O
ATOM	1610	C	ASP	A	218	9.619	20.566	14.610	1.00	11.30	A	C
ATOM	1611	O	ASP	A	218	10.441	20.772	15.501	1.00	10.85	A	O
ATOM	1612	N	VAL	A	219	9.928	20.516	13.314	1.00	11.61	A	N
ATOM	1613	CA	VAL	A	219	11.254	20.829	12.815	1.00	12.37	A	C
ATOM	1614	CB	VAL	A	219	12.118	19.589	12.602	1.00	12.19	A	C
ATOM	1615	CG1	VAL	A	219	12.401	18.867	13.933	1.00	14.24	A	C
ATOM	1616	CG2	VAL	A	219	11.485	18.660	11.587	1.00	13.54	A	C
ATOM	1617	C	VAL	A	219	11.148	21.568	11.471	1.00	12.33	A	C
ATOM	1618	O	VAL	A	219	10.083	21.624	10.851	1.00	12.34	A	O
ATOM	1619	N	MET	A	220	12.266	22.139	11.057	1.00	11.78	A	N
ATOM	1620	CA	MET	A	220	12.365	22.930	9.852	1.00	11.89	A	C
ATOM	1621	CB	MET	A	220	12.798	24.371	10.167	1.00	11.30	A	C
ATOM	1622	CG	MET	A	220	12.025	25.058	11.255	1.00	11.64	A	C
ATOM	1623	SD	MET	A	220	10.310	25.322	10.860	1.00	12.02	A	S
ATOM	1624	CE	MET	A	220	10.416	26.727	9.791	1.00	11.35	A	C
ATOM	1625	C	MET	A	220	13.398	22.343	8.902	1.00	12.21	A	C
ATOM	1626	O	MET	A	220	14.368	21.731	9.321	1.00	12.24	A	O
ATOM	1627	N	ALA	A	221	13.175	22.556	7.613	1.00	12.60	A	N
ATOM	1628	CA	ALA	A	221	14.198	22.324	6.605	1.00	12.90	A	C
ATOM	1629	CB	ALA	A	221	14.098	20.912	6.081	1.00	12.23	A	C
ATOM	1630	C	ALA	A	221	14.064	23.341	5.464	1.00	13.77	A	C
ATOM	1631	O	ALA	A	221	13.029	24.027	5.312	1.00	14.46	A	O
ATOM	1632	N	PRO	A	222	15.116	23.487	4.687	1.00	13.99	A	N
ATOM	1633	CA	PRO	A	222	15.059	24.393	3.543	1.00	14.73	A	C
ATOM	1634	CB	PRO	A	222	16.387	24.159	2.845	1.00	13.69	A	C
ATOM	1635	CG	PRO	A	222	17.290	23.676	3.892	1.00	15.06	A	C
ATOM	1636	CD	PRO	A	222	16.433	22.855	4.830	1.00	14.39	A	C
ATOM	1637	C	PRO	A	222	13.896	24.044	2.622	1.00	14.82	A	C
ATOM	1638	O	PRO	A	222	13.719	22.847	2.284	1.00	15.21	A	O
ATOM	1639	N	GLY	A	223	13.178	25.069	2.193	1.00	14.57	A	N
ATOM	1640	CA	GLY	A	223	11.996	24.910	1.373	1.00	15.06	A	C
ATOM	1641	C	GLY	A	223	11.779	26.046	0.383	1.00	14.81	A	C
ATOM	1642	O	GLY	A	223	10.661	26.268	-0.039	1.00	15.67	A	O
ATOM	1643	N	THR	A	224	12.822	26.799	0.049	1.00	13.98	A	N
ATOM	1644	CA	THR	A	224	12.706	27.772	-1.007	1.00	14.01	A	C
ATOM	1645	CB	THR	A	224	12.912	29.229	-0.517	1.00	13.98	A	C
ATOM	1646	OG1	THR	A	224	14.220	29.350	0.047	1.00	13.39	A	O
ATOM	1647	CG2	THR	A	224	11.952	29.585	0.597	1.00	14.59	A	C
ATOM	1648	C	THR	A	224	13.729	27.449	-2.072	1.00	14.02	A	C
ATOM	1649	O	THR	A	224	14.813	26.932	-1.791	1.00	14.13	A	O
ATOM	1650	N	TYR	A	225	13.389	27.786	-3.308	1.00	14.73	A	N

ATOM	1651	CA	TYR	A	225	14.270	27.528	-4.441	1.00	14.78	A	C
ATOM	1652	CB	TYR	A	225	15.197	28.726	-4.686	1.00	15.26	A	C
ATOM	1653	CG	TYR	A	225	14.502	29.848	-5.398	1.00	15.90	A	C
ATOM	1654	CD1	TYR	A	225	14.027	30.940	-4.692	1.00	18.12	A	C
ATOM	1655	CE1	TYR	A	225	13.349	31.960	-5.301	1.00	18.57	A	C
ATOM	1656	CZ	TYR	A	225	13.100	31.918	-6.659	1.00	19.46	A	C
ATOM	1657	OH	TYR	A	225	12.391	32.974	-7.207	1.00	20.70	A	O
ATOM	1658	CE2	TYR	A	225	13.510	30.844	-7.404	1.00	18.30	A	C
ATOM	1659	CD2	TYR	A	225	14.225	29.788	-6.771	1.00	19.15	A	C
ATOM	1660	C	TYR	A	225	15.022	26.196	-4.331	1.00	14.79	A	C
ATOM	1661	O	TYR	A	225	16.252	26.119	-4.395	1.00	15.52	A	O
ATOM	1662	N	ILE	A	226	14.248	25.130	-4.186	1.00	15.07	A	N
ATOM	1663	CA	ILE	A	226	14.773	23.759	-4.155	1.00	14.45	A	C
ATOM	1664	CB	ILE	A	226	13.904	22.866	-3.254	1.00	14.35	A	C
ATOM	1665	CG1	ILE	A	226	13.906	23.341	-1.789	1.00	15.47	A	C
ATOM	1666	CD1	ILE	A	226	15.239	23.250	-1.085	1.00	16.51	A	C
ATOM	1667	CG2	ILE	A	226	14.312	21.400	-3.377	1.00	14.04	A	C
ATOM	1668	C	ILE	A	226	14.780	23.205	-5.580	1.00	14.24	A	C
ATOM	1669	O	ILE	A	226	13.778	23.188	-6.245	1.00	13.78	A	O
ATOM	1670	N	LEU	A	227	15.937	22.753	-6.022	1.00	14.94	A	N
ATOM	1671	CA	LEU	A	227	16.141	22.230	-7.359	1.00	14.97	A	C
ATOM	1672	CB	LEU	A	227	17.541	22.653	-7.827	1.00	15.61	A	C
ATOM	1673	CG	LEU	A	227	17.950	22.137	-9.196	1.00	16.60	A	C
ATOM	1674	CD1	LEU	A	227	16.899	22.508	-10.231	1.00	16.90	A	C
ATOM	1675	CD2	LEU	A	227	19.340	22.669	-9.559	1.00	18.98	A	C
ATOM	1676	C	LEU	A	227	16.010	20.708	-7.284	1.00	14.76	A	C
ATOM	1677	O	LEU	A	227	16.803	20.038	-6.602	1.00	15.34	A	O
ATOM	1678	N	SER	A	228	14.970	20.179	-7.924	1.00	14.03	A	N
ATOM	1679	CA	SER	A	228	14.665	18.752	-7.871	1.00	14.07	A	C
ATOM	1680	CB	SER	A	228	13.701	18.448	-6.701	1.00	13.81	A	C
ATOM	1681	OG	SER	A	228	13.631	17.038	-6.453	1.00	12.38	A	O
ATOM	1682	C	SER	A	228	14.061	18.319	-9.208	1.00	14.98	A	C
ATOM	1683	O	SER	A	228	13.971	19.115	-10.133	1.00	15.43	A	O
ATOM	1684	N	ALA	A	229	13.626	17.067	-9.278	1.00	14.57	A	N
ATOM	1685	CA	ALA	A	229	13.155	16.454	-10.516	1.00	14.87	A	C
ATOM	1686	CB	ALA	A	229	12.824	14.945	-10.268	1.00	14.78	A	C
ATOM	1687	C	ALA	A	229	11.939	17.135	-11.086	1.00	14.83	A	C
ATOM	1688	O	ALA	A	229	10.939	17.411	-10.376	1.00	14.22	A	O
ATOM	1689	N	ARG	A	230	12.027	17.381	-12.394	1.00	14.42	A	N
ATOM	1690	CA	ARG	A	230	10.974	18.013	-13.155	1.00	14.49	A	C
ATOM	1691	CB	ARG	A	230	11.553	19.008	-14.137	1.00	14.60	A	C
ATOM	1692	CG	ARG	A	230	10.516	19.626	-15.065	1.00	16.55	A	C
ATOM	1693	CD	ARG	A	230	11.044	20.792	-15.934	1.00	19.98	A	C
ATOM	1694	NE	ARG	A	230	9.940	21.308	-16.751	1.00	19.63	A	N
ATOM	1695	CZ	ARG	A	230	9.692	22.581	-16.995	1.00	21.34	A	C
ATOM	1696	NH1	ARG	A	230	10.502	23.547	-16.545	1.00	21.55	A	N
ATOM	1697	NH2	ARG	A	230	8.617	22.898	-17.730	1.00	20.71	A	N
ATOM	1698	C	ARG	A	230	10.232	16.947	-13.948	1.00	14.81	A	C
ATOM	1699	O	ARG	A	230	10.838	16.237	-14.762	1.00	14.40	A	O
ATOM	1700	N	SER	A	231	8.931	16.837	-13.703	1.00	14.68	A	N
ATOM	1701	CA	SER	A	231	8.106	15.937	-14.463	1.00	15.32	A	C
ATOM	1702	CB	SER	A	231	6.660	16.034	-14.030	1.00	15.75	A	C
ATOM	1703	OG	SER	A	231	5.836	15.317	-14.947	1.00	16.08	A	O
ATOM	1704	C	SER	A	231	8.176	16.325	-15.956	1.00	15.44	A	C
ATOM	1705	O	SER	A	231	8.087	17.494	-16.306	1.00	13.31	A	O
ATOM	1706	N	SER	A	232	8.295	15.321	-16.802	1.00	15.69	A	N
ATOM	1707	CA	SER	A	232	8.323	15.494	-18.255	1.00	16.52	A	C
ATOM	1708	CB	SER	A	232	8.682	14.156	-18.906	1.00	16.29	A	C



ATOM	1709	OG	SER	A	232	7.610	13.191	-18.730	1.00	16.72	A	O
ATOM	1710	C	SER	A	232	7.004	16.050	-18.820	1.00	18.10	A	C
ATOM	1711	O	SER	A	232	6.970	16.540	-19.945	1.00	18.08	A	O
ATOM	1712	N	LEU	A	233	5.924	16.005	-18.040	1.00	18.99	A	N
ATOM	1713	CA	LEU	A	233	4.647	16.550	-18.466	1.00	19.87	A	C
ATOM	1714	CB	LEU	A	233	3.503	15.655	-17.989	1.00	20.52	A	C
ATOM	1715	CG	LEU	A	233	3.579	14.202	-18.428	1.00	22.45	A	C
ATOM	1716	CD1	LEU	A	233	2.344	13.472	-17.943	1.00	25.84	A	C
ATOM	1717	CD2	LEU	A	233	3.683	14.146	-19.948	1.00	26.24	A	C
ATOM	1718	C	LEU	A	233	4.357	17.956	-17.940	1.00	20.22	A	C
ATOM	1719	O	LEU	A	233	3.365	18.546	-18.345	1.00	20.30	A	O
ATOM	1720	N	ALA	A	234	5.164	18.485	-17.016	1.00	18.84	A	N
ATOM	1721	CA	ALA	A	234	4.768	19.731	-16.365	1.00	19.34	A	C
ATOM	1722	CB	ALA	A	234	5.297	19.781	-14.958	1.00	18.58	A	C
ATOM	1723	C	ALA	A	234	5.197	20.991	-17.153	1.00	19.93	A	C
ATOM	1724	O	ALA	A	234	6.300	21.037	-17.701	1.00	20.41	A	O
ATOM	1725	N	PRO	A	235	4.325	21.989	-17.197	1.00	20.75	A	N
ATOM	1726	CA	PRO	A	235	4.642	23.288	-17.802	1.00	21.88	A	C
ATOM	1727	CB	PRO	A	235	3.271	23.921	-17.981	1.00	21.83	A	C
ATOM	1728	CG	PRO	A	235	2.429	23.326	-16.902	1.00	21.93	A	C
ATOM	1729	CD	PRO	A	235	2.947	21.944	-16.677	1.00	21.22	A	C
ATOM	1730	C	PRO	A	235	5.495	24.199	-16.885	1.00	22.70	A	C
ATOM	1731	O	PRO	A	235	5.513	23.970	-15.671	1.00	21.06	A	O
ATOM	1732	N	ASP	A	236	6.150	25.204	-17.489	1.00	24.00	A	N
ATOM	1733	CA	ASP	A	236	6.960	26.228	-16.795	1.00	24.41	A	C
ATOM	1734	CB	ASP	A	236	7.455	27.332	-17.750	1.00	24.21	A	C
ATOM	1735	CG	ASP	A	236	8.603	26.838	-18.636	1.00	25.42	A	C
ATOM	1736	OD1	ASP	A	236	9.214	27.656	-19.365	1.00	25.18	A	O
ATOM	1737	OD2	ASP	A	236	8.990	25.634	-18.674	1.00	23.87	A	O
ATOM	1738	C	ASP	A	236	6.263	26.644	-15.520	1.00	24.33	A	C
ATOM	1739	O	ASP	A	236	6.919	27.035	-14.558	1.00	24.16	A	O
ATOM	1740	N	SER	A	237	4.933	26.677	-15.491	1.00	25.32	A	N
ATOM	1741	CA	SER	A	237	4.179	27.723	-14.873	1.00	24.89	A	C
ATOM	1742	CB	SER	A	237	2.801	27.926	-15.490	1.00	25.98	A	C
ATOM	1743	OG	SER	A	237	2.035	26.723	-15.436	1.00	27.95	A	O
ATOM	1744	C	SER	A	237	4.027	26.960	-13.487	1.00	24.14	A	C
ATOM	1745	O	SER	A	237	3.588	27.516	-12.495	1.00	23.01	A	O
ATOM	1746	N	SER	A	238	4.363	25.660	-13.448	1.00	22.59	A	N
ATOM	1747	CA	SER	A	238	4.313	24.861	-12.201	1.00	22.41	A	C
ATOM	1748	CB	SER	A	238	4.238	23.344	-12.501	1.00	22.11	A	C
ATOM	1749	OG	SER	A	238	3.046	22.968	-13.146	1.00	22.38	A	O
ATOM	1750	C	SER	A	238	5.543	25.045	-11.295	1.00	21.86	A	C
ATOM	1751	O	SER	A	238	5.550	24.542	-10.184	1.00	22.29	A	O
ATOM	1752	N	PHE	A	239	6.568	25.744	-11.789	1.00	21.32	A	N
ATOM	1753	CA	PHE	A	239	7.847	25.899	-11.108	1.00	20.67	A	C
ATOM	1754	CB	PHE	A	239	8.966	25.299	-11.966	1.00	20.17	A	C
ATOM	1755	CG	PHE	A	239	8.736	23.854	-12.294	1.00	20.18	A	C
ATOM	1756	CD1	PHE	A	239	8.964	22.881	-11.344	1.00	18.34	A	C
ATOM	1757	CE1	PHE	A	239	8.686	21.573	-11.600	1.00	15.67	A	C
ATOM	1758	CZ	PHE	A	239	8.194	21.184	-12.814	1.00	16.81	A	C
ATOM	1759	CE2	PHE	A	239	7.924	22.128	-13.775	1.00	16.81	A	C
ATOM	1760	CD2	PHE	A	239	8.194	23.466	-13.520	1.00	18.63	A	C
ATOM	1761	C	PHE	A	239	8.124	27.370	-10.775	1.00	20.81	A	C
ATOM	1762	O	PHE	A	239	7.589	28.283	-11.404	1.00	19.94	A	O
ATOM	1763	N	TRP	A	240	8.927	27.575	-9.743	1.00	20.46	A	N
ATOM	1764	CA	TRP	A	240	9.420	28.913	-9.382	1.00	21.13	A	C
ATOM	1765	CB	TRP	A	240	10.192	28.842	-8.055	1.00	21.05	A	C
ATOM	1766	CG	TRP	A	240	9.324	28.850	-6.857	1.00	22.76	A	C



ATOM	1767	CD1	TRP	A	240	8.027	28.446	-6.782	1.00	23.97	A	C
ATOM	1768	NE1	TRP	A	240	7.548	28.624	-5.509	1.00	24.62	A	N
ATOM	1769	CE2	TRP	A	240	8.547	29.148	-4.726	1.00	24.31	A	C
ATOM	1770	CD2	TRP	A	240	9.677	29.302	-5.537	1.00	23.24	A	C
ATOM	1771	CE3	TRP	A	240	10.839	29.811	-4.966	1.00	24.95	A	C
ATOM	1772	CZ3	TRP	A	240	10.833	30.146	-3.637	1.00	24.14	A	C
ATOM	1773	CH2	TRP	A	240	9.682	29.991	-2.857	1.00	23.89	A	C
ATOM	1774	CZ2	TRP	A	240	8.542	29.483	-3.378	1.00	25.05	A	C
ATOM	1775	C	TRP	A	240	10.355	29.466	-10.461	1.00	20.95	A	C
ATOM	1776	O	TRP	A	240	10.419	30.673	-10.703	1.00	20.42	A	O
ATOM	1777	N	ALA	A	241	11.097	28.566	-11.080	1.00	21.11	A	N
ATOM	1778	CA	ALA	A	241	12.022	28.907	-12.149	1.00	21.52	A	C
ATOM	1779	CB	ALA	A	241	13.243	29.629	-11.606	1.00	21.93	A	C
ATOM	1780	C	ALA	A	241	12.466	27.641	-12.801	1.00	21.79	A	C
ATOM	1781	O	ALA	A	241	12.440	26.569	-12.169	1.00	22.05	A	O
ATOM	1782	N	ASN	A	242	12.929	27.769	-14.040	1.00	22.09	A	N
ATOM	1783	CA	ASN	A	242	13.481	26.656	-14.800	1.00	22.74	A	C
ATOM	1784	CB	ASN	A	242	13.397	26.962	-16.322	1.00	22.69	A	C
ATOM	1785	CG	ASN	A	242	11.960	27.071	-16.828	1.00	22.96	A	C
ATOM	1786	OD1	ASN	A	242	11.024	26.578	-16.198	1.00	21.33	A	O
ATOM	1787	ND2	ASN	A	242	11.782	27.727	-17.969	1.00	21.31	A	N
ATOM	1788	C	ASN	A	242	14.927	26.359	-14.458	1.00	23.18	A	C
ATOM	1789	O	ASN	A	242	15.634	27.194	-13.902	1.00	23.35	A	O
ATOM	1790	N	HIS	A	243	15.375	25.169	-14.820	1.00	24.21	A	N
ATOM	1791	CA	HIS	A	243	16.802	24.875	-14.862	1.00	25.06	A	C
ATOM	1792	CB	HIS	A	243	17.234	24.062	-13.653	1.00	25.31	A	C
ATOM	1793	CG	HIS	A	243	18.703	23.809	-13.595	1.00	27.16	A	C
ATOM	1794	ND1	HIS	A	243	19.599	24.733	-13.086	1.00	30.11	A	N
ATOM	1795	CE1	HIS	A	243	20.820	24.231	-13.152	1.00	30.29	A	C
ATOM	1796	NE2	HIS	A	243	20.752	23.036	-13.713	1.00	29.63	A	N
ATOM	1797	CD2	HIS	A	243	19.442	22.754	-14.008	1.00	28.73	A	C
ATOM	1798	C	HIS	A	243	17.158	24.144	-16.162	1.00	26.02	A	C
ATOM	1799	O	HIS	A	243	17.851	24.726	-17.003	1.00	25.77	A	O
ATOM	1800	N	ASP	A	244	16.711	22.880	-16.299	1.00	26.20	A	N
ATOM	1801	CA	ASP	A	244	16.757	22.137	-17.584	1.00	27.35	A	C
ATOM	1802	CB	ASP	A	244	17.972	21.252	-17.646	1.00	28.02	A	C
ATOM	1803	CG	ASP	A	244	18.211	20.272	-16.546	1.00	29.28	A	C
ATOM	1804	OD1	ASP	A	244	19.393	20.188	-16.099	1.00	34.73	A	O
ATOM	1805	OD2	ASP	A	244	17.310	19.568	-16.056	1.00	28.43	A	O
ATOM	1806	C	ASP	A	244	15.427	21.429	-17.760	1.00	27.57	A	C
ATOM	1807	O	ASP	A	244	14.751	21.208	-16.721	1.00	27.11	A	O
ATOM	1808	N	SER	A	245	15.290	20.734	-18.836	1.00	27.83	A	N
ATOM	1809	CA	SER	A	245	14.559	19.557	-19.209	1.00	26.73	A	C
ATOM	1810	CB	SER	A	245	15.083	18.972	-20.483	1.00	26.99	A	C
ATOM	1811	OG	SER	A	245	15.792	17.785	-20.481	1.00	27.12	A	O
ATOM	1812	C	SER	A	245	14.234	18.594	-18.102	1.00	25.28	A	C
ATOM	1813	O	SER	A	245	13.146	17.973	-18.152	1.00	24.66	A	O
ATOM	1814	N	LYS	A	246	15.122	18.339	-17.176	1.00	23.51	A	N
ATOM	1815	CA	LYS	A	246	14.918	17.304	-16.177	1.00	22.90	A	C
ATOM	1816	CB	LYS	A	246	15.977	16.205	-16.332	1.00	23.64	A	C
ATOM	1817	CG	LYS	A	246	15.852	15.384	-17.600	1.00	26.42	A	C
ATOM	1818	CD	LYS	A	246	17.094	14.548	-17.859	1.00	29.39	A	C
ATOM	1819	CE	LYS	A	246	16.880	13.584	-19.018	1.00	32.94	A	C
ATOM	1820	NZ	LYS	A	246	18.070	13.501	-19.908	1.00	37.30	A	N
ATOM	1821	C	LYS	A	246	14.812	17.762	-14.740	1.00	21.77	A	C
ATOM	1822	O	LYS	A	246	14.396	17.059	-13.828	1.00	19.24	A	O
ATOM	1823	N	TYR	A	247	15.126	19.026	-14.452	1.00	20.43	A	N
ATOM	1824	CA	TYR	A	247	15.144	19.544	-13.079	1.00	19.83	A	C

ATOM	1825	CB	TYR	A	247	16.541	19.398	-12.456	1.00	19.35	A	C
ATOM	1826	CG	TYR	A	247	17.007	17.966	-12.434	1.00	19.14	A	C
ATOM	1827	CD1	TYR	A	247	17.784	17.442	-13.482	1.00	21.08	A	C
ATOM	1828	CE1	TYR	A	247	18.170	16.121	-13.489	1.00	17.97	A	C
ATOM	1829	CZ	TYR	A	247	17.780	15.292	-12.458	1.00	19.97	A	C
ATOM	1830	OH	TYR	A	247	18.159	13.964	-12.465	1.00	18.06	A	O
ATOM	1831	CE2	TYR	A	247	16.999	15.781	-11.417	1.00	18.19	A	C
ATOM	1832	CD2	TYR	A	247	16.630	17.109	-11.408	1.00	19.09	A	C
ATOM	1833	C	TYR	A	247	14.697	21.003	-13.069	1.00	18.89	A	C
ATOM	1834	O	TYR	A	247	15.017	21.761	-13.994	1.00	18.71	A	O
ATOM	1835	N	ALA	A	248	13.936	21.385	-12.046	1.00	17.07	A	N
ATOM	1836	CA	ALA	A	248	13.512	22.769	-11.893	1.00	16.28	A	C
ATOM	1837	CB	ALA	A	248	12.294	23.035	-12.733	1.00	15.85	A	C
ATOM	1838	C	ALA	A	248	13.253	23.110	-10.425	1.00	15.75	A	C
ATOM	1839	O	ALA	A	248	13.358	22.236	-9.549	1.00	15.81	A	O
ATOM	1840	N	TYR	A	249	12.956	24.384	-10.174	1.00	15.33	A	N
ATOM	1841	CA	TYR	A	249	12.910	24.949	-8.832	1.00	15.08	A	C
ATOM	1842	CB	TYR	A	249	13.520	26.336	-8.802	1.00	15.54	A	C
ATOM	1843	CG	TYR	A	249	14.999	26.398	-9.087	1.00	15.33	A	C
ATOM	1844	CD1	TYR	A	249	15.470	26.675	-10.370	1.00	17.29	A	C
ATOM	1845	CE1	TYR	A	249	16.829	26.754	-10.640	1.00	16.19	A	C
ATOM	1846	CZ	TYR	A	249	17.741	26.557	-9.608	1.00	18.72	A	C
ATOM	1847	OH	TYR	A	249	19.088	26.649	-9.839	1.00	21.92	A	O
ATOM	1848	CE2	TYR	A	249	17.306	26.287	-8.330	1.00	18.20	A	C
ATOM	1849	CD2	TYR	A	249	15.930	26.207	-8.070	1.00	17.03	A	C
ATOM	1850	C	TYR	A	249	11.497	25.078	-8.358	1.00	15.50	A	C
ATOM	1851	O	TYR	A	249	10.599	25.480	-9.122	1.00	16.06	A	O
ATOM	1852	N	MET	A	250	11.291	24.749	-7.082	1.00	15.10	A	N
ATOM	1853	CA	MET	A	250	10.015	24.967	-6.430	1.00	15.40	A	C
ATOM	1854	CB	MET	A	250	9.153	23.703	-6.542	1.00	15.90	A	C
ATOM	1855	CG	MET	A	250	7.677	23.947	-6.729	1.00	19.64	A	C
ATOM	1856	SD	MET	A	250	6.677	22.370	-6.869	1.00	23.44	A	S
ATOM	1857	CE	MET	A	250	7.321	21.709	-8.163	1.00	22.96	A	C
ATOM	1858	C	MET	A	250	10.274	25.318	-4.966	1.00	15.09	A	C
ATOM	1859	O	MET	A	250	11.366	25.081	-4.440	1.00	15.78	A	O
ATOM	1860	N	GLY	A	251	9.279	25.888	-4.314	1.00	14.69	A	N
ATOM	1861	CA	GLY	A	251	9.373	26.203	-2.902	1.00	13.76	A	C
ATOM	1862	C	GLY	A	251	8.026	26.058	-2.248	1.00	14.49	A	C
ATOM	1863	O	GLY	A	251	6.984	26.057	-2.933	1.00	13.60	A	O
ATOM	1864	N	GLY	A	252	8.056	25.926	-0.920	1.00	12.84	A	N
ATOM	1865	CA	GLY	A	252	6.879	25.694	-0.101	1.00	13.22	A	C
ATOM	1866	C	GLY	A	252	7.242	24.765	1.058	1.00	12.42	A	C
ATOM	1867	O	GLY	A	252	8.354	24.185	1.073	1.00	11.46	A	O
ATOM	1868	N	THR	A	253	6.328	24.598	2.008	1.00	12.37	A	N
ATOM	1869	CA	THR	A	253	6.518	23.583	3.043	1.00	12.51	A	C
ATOM	1870	CB	THR	A	253	5.543	23.697	4.256	1.00	13.05	A	C
ATOM	1871	OG1	THR	A	253	4.138	23.788	3.858	1.00	11.78	A	O
ATOM	1872	CG2	THR	A	253	5.837	24.964	5.042	1.00	13.23	A	C
ATOM	1873	C	THR	A	253	6.463	22.211	2.396	1.00	12.60	A	C
ATOM	1874	O	THR	A	253	6.945	21.239	2.966	1.00	12.54	A	O
ATOM	1875	N	SER	A	254	5.902	22.158	1.187	1.00	12.69	A	N
ATOM	1876	CA	SER	A	254	5.905	20.957	0.357	1.00	12.54	A	C
ATOM	1877	CB	SER	A	254	5.228	21.233	-0.994	1.00	12.41	A	C
ATOM	1878	OG	SER	A	254	3.822	21.002	-0.960	1.00	11.90	A	O
ATOM	1879	C	SER	A	254	7.298	20.445	0.050	1.00	12.52	A	C
ATOM	1880	O	SER	A	254	7.459	19.253	-0.150	1.00	12.45	A	O
ATOM	1881	N	MET	A	255	8.255	21.361	-0.054	1.00	12.52	A	N
ATOM	1882	CA	MET	A	255	9.640	21.062	-0.385	1.00	13.23	A	C

ATOM	1883	CB	MET	A	255	10.260	22.231	-1.164	1.00	13.16	A	C
ATOM	1884	CG	MET	A	255	9.955	22.255	-2.667	1.00	13.61	A	C
ATOM	1885	SD	MET	A	255	8.220	22.693	-3.027	1.00	16.25	A	S
ATOM	1886	CE	MET	A	255	7.683	21.071	-3.591	1.00	13.35	A	C
ATOM	1887	C	MET	A	255	10.478	20.759	0.873	1.00	13.32	A	C
ATOM	1888	O	MET	A	255	11.396	19.934	0.847	1.00	13.21	A	O
ATOM	1889	N	ALA	A	256	10.162	21.415	1.981	1.00	12.98	A	N
ATOM	1890	CA	ALA	A	256	10.904	21.161	3.213	1.00	12.47	A	C
ATOM	1891	CB	ALA	A	256	10.516	22.175	4.265	1.00	11.99	A	C
ATOM	1892	C	ALA	A	256	10.645	19.737	3.717	1.00	11.89	A	C
ATOM	1893	O	ALA	A	256	11.553	19.018	4.179	1.00	11.48	A	O
ATOM	1894	N	THR	A	257	9.390	19.341	3.629	1.00	11.55	A	N
ATOM	1895	CA	THR	A	257	8.944	18.065	4.146	1.00	11.50	A	C
ATOM	1896	CB	THR	A	257	7.423	17.938	3.908	1.00	12.07	A	C
ATOM	1897	OG1	THR	A	257	6.754	19.013	4.569	1.00	13.08	A	O
ATOM	1898	CG2	THR	A	257	6.838	16.661	4.540	1.00	12.46	A	C
ATOM	1899	C	THR	A	257	9.705	16.849	3.587	1.00	11.20	A	C
ATOM	1900	O	THR	A	257	10.172	16.018	4.382	1.00	11.03	A	O
ATOM	1901	N	PRO	A	258	9.781	16.686	2.259	1.00	11.22	A	N
ATOM	1902	CA	PRO	A	258	10.466	15.521	1.687	1.00	10.92	A	C
ATOM	1903	CB	PRO	A	258	10.200	15.644	0.182	1.00	10.45	A	C
ATOM	1904	CG	PRO	A	258	9.884	17.057	-0.029	1.00	11.62	A	C
ATOM	1905	CD	PRO	A	258	9.164	17.504	1.207	1.00	10.92	A	C
ATOM	1906	C	PRO	A	258	11.969	15.503	1.976	1.00	10.83	A	C
ATOM	1907	O	PRO	A	258	12.524	14.417	2.020	1.00	9.95	A	O
ATOM	1908	N	ILE	A	259	12.605	16.665	2.160	1.00	11.19	A	N
ATOM	1909	CA	ILE	A	259	14.004	16.711	2.597	1.00	11.51	A	C
ATOM	1910	CB	ILE	A	259	14.439	18.183	2.712	1.00	11.81	A	C
ATOM	1911	CG1	ILE	A	259	14.492	18.843	1.314	1.00	14.15	A	C
ATOM	1912	CD1	ILE	A	259	15.690	18.403	0.504	1.00	17.31	A	C
ATOM	1913	CG2	ILE	A	259	15.790	18.313	3.375	1.00	11.02	A	C
ATOM	1914	C	ILE	A	259	14.147	15.975	3.950	1.00	11.56	A	C
ATOM	1915	O	ILE	A	259	15.038	15.133	4.124	1.00	11.81	A	O
ATOM	1916	N	VAL	A	260	13.259	16.295	4.886	1.00	11.02	A	N
ATOM	1917	CA	VAL	A	260	13.244	15.668	6.199	1.00	12.26	A	C
ATOM	1918	CB	VAL	A	260	12.301	16.412	7.150	1.00	12.30	A	C
ATOM	1919	CG1	VAL	A	260	12.286	15.743	8.557	1.00	12.78	A	C
ATOM	1920	CG2	VAL	A	260	12.721	17.855	7.268	1.00	13.51	A	C
ATOM	1921	C	VAL	A	260	12.847	14.185	6.106	1.00	12.24	A	C
ATOM	1922	O	VAL	A	260	13.412	13.339	6.786	1.00	12.79	A	O
ATOM	1923	N	ALA	A	261	11.922	13.864	5.217	1.00	12.41	A	N
ATOM	1924	CA	ALA	A	261	11.530	12.480	4.997	1.00	11.93	A	C
ATOM	1925	CB	ALA	A	261	10.426	12.376	3.920	1.00	12.16	A	C
ATOM	1926	C	ALA	A	261	12.750	11.661	4.585	1.00	11.91	A	C
ATOM	1927	O	ALA	A	261	12.943	10.560	5.055	1.00	11.34	A	O
ATOM	1928	N	GLY	A	262	13.550	12.186	3.665	1.00	12.22	A	N
ATOM	1929	CA	GLY	A	262	14.794	11.533	3.291	1.00	12.29	A	C
ATOM	1930	C	GLY	A	262	15.786	11.431	4.447	1.00	12.34	A	C
ATOM	1931	O	GLY	A	262	16.414	10.386	4.660	1.00	11.90	A	O
ATOM	1932	N	ASN	A	263	15.901	12.490	5.243	1.00	12.20	A	N
ATOM	1933	CA	ASN	A	263	16.744	12.433	6.435	1.00	11.84	A	C
ATOM	1934	CB	ASN	A	263	16.772	13.773	7.170	1.00	12.31	A	C
ATOM	1935	CG	ASN	A	263	17.389	14.887	6.351	1.00	13.12	A	C
ATOM	1936	OD1	ASN	A	263	18.326	14.681	5.525	1.00	15.95	A	O
ATOM	1937	ND2	ASN	A	263	16.924	16.073	6.600	1.00	9.15	A	N
ATOM	1938	C	ASN	A	263	16.289	11.348	7.396	1.00	11.83	A	C
ATOM	1939	O	ASN	A	263	17.112	10.672	8.020	1.00	11.88	A	O
ATOM	1940	N	VAL	A	264	14.983	11.181	7.517	1.00	11.77	A	N

ATOM	1941	CA	VAL	A	264	14.425	10.138	8.367	1.00	12.33	A	C
ATOM	1942	CB	VAL	A	264	12.893	10.268	8.506	1.00	12.44	A	C
ATOM	1943	CG1	VAL	A	264	12.280	9.045	9.178	1.00	12.44	A	C
ATOM	1944	CG2	VAL	A	264	12.543	11.471	9.323	1.00	13.22	A	C
ATOM	1945	C	VAL	A	264	14.817	8.754	7.843	1.00	11.95	A	C
ATOM	1946	O	VAL	A	264	15.164	7.896	8.625	1.00	12.24	A	O
ATOM	1947	N	ALA	A	265	14.813	8.553	6.527	1.00	12.03	A	N
ATOM	1948	CA	ALA	A	265	15.279	7.292	5.966	1.00	11.47	A	C
ATOM	1949	CB	ALA	A	265	15.018	7.237	4.460	1.00	11.96	A	C
ATOM	1950	C	ALA	A	265	16.746	7.046	6.293	1.00	11.77	A	C
ATOM	1951	O	ALA	A	265	17.139	5.932	6.592	1.00	11.77	A	O
ATOM	1952	N	GLN	A	266	17.571	8.091	6.262	1.00	12.48	A	N
ATOM	1953	CA	GLN	A	266	18.999	7.940	6.586	1.00	11.99	A	C
ATOM	1954	CB	GLN	A	266	19.782	9.230	6.311	1.00	10.90	A	C
ATOM	1955	CG	GLN	A	266	19.786	9.691	4.865	1.00	12.48	A	C
ATOM	1956	CD	GLN	A	266	20.548	11.011	4.671	1.00	12.24	A	C
ATOM	1957	OE1	GLN	A	266	21.762	11.028	4.352	1.00	16.02	A	O
ATOM	1958	NE2	GLN	A	266	19.857	12.088	4.853	1.00	8.53	A	N
ATOM	1959	C	GLN	A	266	19.159	7.571	8.046	1.00	12.14	A	C
ATOM	1960	O	GLN	A	266	19.927	6.688	8.398	1.00	12.13	A	O
ATOM	1961	N	LEU	A	267	18.463	8.305	8.898	1.00	12.44	A	N
ATOM	1962	CA	LEU	A	267	18.473	8.049	10.317	1.00	12.06	A	C
ATOM	1963	CB	LEU	A	267	17.624	9.107	11.014	1.00	12.45	A	C
ATOM	1964	CG	LEU	A	267	17.550	9.097	12.540	1.00	12.15	A	C
ATOM	1965	CD1	LEU	A	267	18.918	9.293	13.116	1.00	12.99	A	C
ATOM	1966	CD2	LEU	A	267	16.616	10.187	13.009	1.00	12.84	A	C
ATOM	1967	C	LEU	A	267	17.984	6.649	10.654	1.00	12.72	A	C
ATOM	1968	O	LEU	A	267	18.581	5.972	11.497	1.00	12.91	A	O
ATOM	1969	N	ARG	A	268	16.872	6.219	10.044	1.00	12.54	A	N
ATOM	1970	CA	ARG	A	268	16.295	4.886	10.321	1.00	12.31	A	C
ATOM	1971	CB	ARG	A	268	14.961	4.722	9.577	1.00	12.21	A	C
ATOM	1972	CG	ARG	A	268	14.016	3.635	10.155	1.00	12.56	A	C
ATOM	1973	CD	ARG	A	268	12.652	3.605	9.510	1.00	14.20	A	C
ATOM	1974	NE	ARG	A	268	11.781	2.591	10.105	1.00	14.70	A	N
ATOM	1975	CZ	ARG	A	268	11.837	1.306	9.829	1.00	14.81	A	C
ATOM	1976	NH1	ARG	A	268	12.697	0.829	8.942	1.00	14.11	A	N
ATOM	1977	NH2	ARG	A	268	10.993	0.483	10.432	1.00	15.99	A	N
ATOM	1978	C	ARG	A	268	17.284	3.763	9.929	1.00	12.37	A	C
ATOM	1979	O	ARG	A	268	17.533	2.837	10.689	1.00	11.86	A	O
ATOM	1980	N	GLU	A	269	17.846	3.870	8.729	1.00	11.97	A	N
ATOM	1981	CA	GLU	A	269	18.965	3.026	8.306	1.00	12.12	A	C
ATOM	1982	CB	GLU	A	269	19.561	3.537	6.993	1.00	11.36	A	C
ATOM	1983	CG	GLU	A	269	20.764	2.715	6.542	1.00	12.78	A	C
ATOM	1984	CD	GLU	A	269	21.477	3.260	5.335	1.00	15.24	A	C
ATOM	1985	OE1	GLU	A	269	21.277	4.447	5.007	1.00	16.05	A	O
ATOM	1986	OE2	GLU	A	269	22.246	2.479	4.711	1.00	16.25	A	O
ATOM	1987	C	GLU	A	269	20.082	2.954	9.354	1.00	12.56	A	C
ATOM	1988	O	GLU	A	269	20.596	1.875	9.645	1.00	12.26	A	O
ATOM	1989	N	HIS	A	270	20.482	4.104	9.894	1.00	12.79	A	N
ATOM	1990	CA	HIS	A	270	21.556	4.119	10.859	1.00	12.79	A	C
ATOM	1991	CB	HIS	A	270	21.918	5.531	11.289	1.00	12.76	A	C
ATOM	1992	CG	BHIS	A	270	23.160	5.583	12.120	0.50	10.01	A	C
ATOM	1993	CG	AHIS	A	270	23.195	5.601	12.063	0.50	15.58	A	C
ATOM	1994	ND1	BHIS	A	270	23.186	6.137	13.385	0.50	7.23	A	N
ATOM	1995	ND1	AHIS	A	270	23.243	5.459	13.432	0.50	20.08	A	N
ATOM	1996	CE1	BHIS	A	270	24.404	6.019	13.885	0.50	6.26	A	C
ATOM	1997	CE1	AHIS	A	270	24.498	5.548	13.839	0.50	20.34	A	C
ATOM	1998	NE2	BHIS	A	270	25.163	5.387	13.000	0.50	8.61	A	N



ATOM	1999	NE2AHIS	A	270	25.265	5.744	12.783	0.50	20.61	A	N	
ATOM	2000	CD2BHIS	A	270	24.405	5.102	11.888	0.50	6.18	A	C	
ATOM	2001	CD2AHIS	A	270	24.475	5.782	11.659	0.50	18.53	A	C	
ATOM	2002	C	HIS	A	270	21.210	3.294	12.099	1.00	12.75	A	C
ATOM	2003	O	HIS	A	270	22.031	2.541	12.562	1.00	12.88	A	O
ATOM	2004	N	PHE	A	271	20.009	3.468	12.666	1.00	12.25	A	N
ATOM	2005	CA	PHE	A	271	19.642	2.680	13.834	1.00	12.36	A	C
ATOM	2006	CB	PHE	A	271	18.274	3.114	14.370	1.00	12.01	A	C
ATOM	2007	CG	PHE	A	271	18.328	4.292	15.293	1.00	11.54	A	C
ATOM	2008	CD1	PHE	A	271	18.557	4.127	16.643	1.00	12.44	A	C
ATOM	2009	CE1	PHE	A	271	18.601	5.229	17.500	1.00	13.55	A	C
ATOM	2010	CZ	PHE	A	271	18.400	6.479	17.016	1.00	11.92	A	C
ATOM	2011	CE2	PHE	A	271	18.145	6.655	15.663	1.00	15.14	A	C
ATOM	2012	CD2	PHE	A	271	18.096	5.567	14.820	1.00	13.90	A	C
ATOM	2013	C	PHE	A	271	19.620	1.178	13.492	1.00	13.05	A	C
ATOM	2014	O	PHE	A	271	20.147	0.341	14.240	1.00	15.06	A	O
ATOM	2015	N	VAL	A	272	19.007	0.850	12.371	1.00	12.88	A	N
ATOM	2016	CA	VAL	A	272	18.765	-0.526	11.961	1.00	13.79	A	C
ATOM	2017	CB	VAL	A	272	17.856	-0.539	10.706	1.00	13.45	A	C
ATOM	2018	CG1	VAL	A	272	17.977	-1.840	9.953	1.00	15.25	A	C
ATOM	2019	CG2	VAL	A	272	16.429	-0.264	11.112	1.00	13.55	A	C
ATOM	2020	C	VAL	A	272	20.068	-1.276	11.689	1.00	14.17	A	C
ATOM	2021	O	VAL	A	272	20.242	-2.415	12.162	1.00	14.67	A	O
ATOM	2022	N	LYS	A	273	20.992	-0.619	10.990	1.00	14.25	A	N
ATOM	2023	CA	LYS	A	273	22.255	-1.217	10.606	1.00	14.60	A	C
ATOM	2024	CB	LYS	A	273	22.759	-0.664	9.267	1.00	14.93	A	C
ATOM	2025	CG	LYS	A	273	21.893	-1.085	8.052	1.00	15.97	A	C
ATOM	2026	CD	LYS	A	273	22.432	-0.488	6.729	1.00	14.97	A	C
ATOM	2027	CE	LYS	A	273	21.735	-1.010	5.482	1.00	16.43	A	C
ATOM	2028	NZ	LYS	A	273	22.131	-0.162	4.300	1.00	13.02	A	N
ATOM	2029	C	LYS	A	273	23.366	-1.133	11.645	1.00	14.97	A	C
ATOM	2030	O	LYS	A	273	24.172	-2.075	11.740	1.00	12.32	A	O
ATOM	2031	N	ASN	A	274	23.402	-0.033	12.403	1.00	14.72	A	N
ATOM	2032	CA	ASN	A	274	24.556	0.298	13.225	1.00	15.62	A	C
ATOM	2033	CB	ASN	A	274	25.197	1.649	12.786	1.00	16.07	A	C
ATOM	2034	CG	ASN	A	274	25.555	1.662	11.290	1.00	17.59	A	C
ATOM	2035	OD1	ASN	A	274	25.285	2.647	10.543	1.00	18.70	A	O
ATOM	2036	ND2	ASN	A	274	26.124	0.561	10.839	1.00	13.05	A	N
ATOM	2037	C	ASN	A	274	24.253	0.365	14.694	1.00	15.60	A	C
ATOM	2038	O	ASN	A	274	25.165	0.449	15.465	1.00	15.70	A	O
ATOM	2039	N	ARG	A	275	22.979	0.348	15.092	1.00	14.80	A	N
ATOM	2040	CA	ARG	A	275	22.670	0.517	16.505	1.00	15.19	A	C
ATOM	2041	CB	ARG	A	275	22.046	1.883	16.723	1.00	14.89	A	C
ATOM	2042	CG	ARG	A	275	22.925	3.001	16.141	1.00	17.88	A	C
ATOM	2043	CD	ARG	A	275	22.682	4.354	16.748	1.00	17.97	A	C
ATOM	2044	NE	ARG	A	275	23.098	4.391	18.146	1.00	15.44	A	N
ATOM	2045	CZ	ARG	A	275	22.783	5.383	18.977	1.00	18.17	A	C
ATOM	2046	NH1	ARG	A	275	22.080	6.422	18.540	1.00	17.27	A	N
ATOM	2047	NH2	ARG	A	275	23.191	5.356	20.239	1.00	17.72	A	N
ATOM	2048	C	ARG	A	275	21.796	-0.573	17.088	1.00	14.64	A	C
ATOM	2049	O	ARG	A	275	21.382	-0.456	18.212	1.00	15.75	A	O
ATOM	2050	N	GLY	A	276	21.459	-1.577	16.283	1.00	14.66	A	N
ATOM	2051	CA	GLY	A	276	20.880	-2.825	16.771	1.00	14.63	A	C
ATOM	2052	C	GLY	A	276	19.403	-2.811	17.060	1.00	14.40	A	C
ATOM	2053	O	GLY	A	276	18.863	-3.751	17.664	1.00	13.52	A	O
ATOM	2054	N	VAL	A	277	18.729	-1.745	16.638	1.00	14.10	A	N
ATOM	2055	CA	VAL	A	277	17.318	-1.618	16.894	1.00	14.10	A	C
ATOM	2056	CB	VAL	A	277	17.021	-0.657	18.097	1.00	14.71	A	C



ATOM	2057	CG1	VAL	A	277	17.768	-1.058	19.354	1.00	14.49	A	C
ATOM	2058	CG2	VAL	A	277	17.268	0.771	17.733	1.00	15.67	A	C
ATOM	2059	C	VAL	A	277	16.547	-1.097	15.689	1.00	13.79	A	C
ATOM	2060	O	VAL	A	277	17.082	-0.372	14.853	1.00	14.29	A	O
ATOM	2061	N	THR	A	278	15.273	-1.472	15.607	1.00	14.21	A	N
ATOM	2062	CA	THR	A	278	14.325	-0.778	14.749	1.00	14.50	A	C
ATOM	2063	CB	THR	A	278	13.187	-1.700	14.301	1.00	15.23	A	C
ATOM	2064	OG1	THR	A	278	13.744	-2.825	13.607	1.00	19.10	A	O
ATOM	2065	CG2	THR	A	278	12.304	-0.986	13.245	1.00	17.53	A	C
ATOM	2066	C	THR	A	278	13.760	0.394	15.526	1.00	13.49	A	C
ATOM	2067	O	THR	A	278	13.028	0.210	16.485	1.00	13.51	A	O
ATOM	2068	N	PRO	A	279	14.104	1.612	15.134	1.00	12.55	A	N
ATOM	2069	CA	PRO	A	279	13.679	2.803	15.896	1.00	11.32	A	C
ATOM	2070	CB	PRO	A	279	14.520	3.920	15.277	1.00	11.71	A	C
ATOM	2071	CG	PRO	A	279	14.682	3.493	13.842	1.00	11.40	A	C
ATOM	2072	CD	PRO	A	279	14.817	1.975	13.895	1.00	12.28	A	C
ATOM	2073	C	PRO	A	279	12.211	3.055	15.672	1.00	11.90	A	C
ATOM	2074	O	PRO	A	279	11.786	3.053	14.516	1.00	12.19	A	O
ATOM	2075	N	LYS	A	280	11.438	3.212	16.743	1.00	11.50	A	N
ATOM	2076	CA	LYS	A	280	10.020	3.518	16.639	1.00	12.77	A	C
ATOM	2077	CB	LYS	A	280	9.354	3.389	18.024	1.00	13.46	A	C
ATOM	2078	CG	LYS	A	280	9.324	1.993	18.573	1.00	15.21	A	C
ATOM	2079	CD	LYS	A	280	8.273	1.192	17.861	1.00	20.42	A	C
ATOM	2080	CE	LYS	A	280	8.012	-0.146	18.555	1.00	23.45	A	C
ATOM	2081	NZ	LYS	A	280	6.935	-0.858	17.808	1.00	26.12	A	N
ATOM	2082	C	LYS	A	280	9.811	4.951	16.120	1.00	11.96	A	C
ATOM	2083	O	LYS	A	280	10.710	5.782	16.200	1.00	13.23	A	O
ATOM	2084	N	PRO	A	281	8.666	5.233	15.512	1.00	12.23	A	N
ATOM	2085	CA	PRO	A	281	8.370	6.608	15.073	1.00	11.69	A	C
ATOM	2086	CB	PRO	A	281	6.897	6.540	14.763	1.00	12.25	A	C
ATOM	2087	CG	PRO	A	281	6.755	5.162	14.210	1.00	12.66	A	C
ATOM	2088	CD	PRO	A	281	7.592	4.300	15.126	1.00	11.87	A	C
ATOM	2089	C	PRO	A	281	8.682	7.678	16.105	1.00	11.94	A	C
ATOM	2090	O	PRO	A	281	9.287	8.708	15.734	1.00	11.60	A	O
ATOM	2091	N	SER	A	282	8.303	7.447	17.374	1.00	11.91	A	N
ATOM	2092	CA	SER	A	282	8.579	8.404	18.442	1.00	11.78	A	C
ATOM	2093	CB	SER	A	282	8.017	7.930	19.789	1.00	11.85	A	C
ATOM	2094	OG	SER	A	282	8.503	6.639	20.117	1.00	12.30	A	O
ATOM	2095	C	SER	A	282	10.049	8.704	18.654	1.00	11.36	A	C
ATOM	2096	O	SER	A	282	10.402	9.835	19.014	1.00	11.10	A	O
ATOM	2097	N	LEU	A	283	10.896	7.696	18.498	1.00	11.81	A	N
ATOM	2098	CA	LEU	A	283	12.332	7.889	18.642	1.00	11.66	A	C
ATOM	2099	CB	LEU	A	283	13.042	6.532	18.856	1.00	11.73	A	C
ATOM	2100	CG	LEU	A	283	14.575	6.628	18.893	1.00	11.60	A	C
ATOM	2101	CD1	LEU	A	283	15.029	7.501	20.001	1.00	10.08	A	C
ATOM	2102	CD2	LEU	A	283	15.180	5.233	19.066	1.00	15.86	A	C
ATOM	2103	C	LEU	A	283	12.953	8.650	17.465	1.00	11.15	A	C
ATOM	2104	O	LEU	A	283	13.812	9.515	17.644	1.00	11.72	A	O
ATOM	2105	N	LEU	A	284	12.575	8.305	16.244	1.00	11.65	A	N
ATOM	2106	CA	LEU	A	284	13.056	9.058	15.088	1.00	10.89	A	C
ATOM	2107	CB	LEU	A	284	12.493	8.470	13.802	1.00	10.71	A	C
ATOM	2108	CG	LEU	A	284	13.010	7.059	13.442	1.00	10.82	A	C
ATOM	2109	CD1	LEU	A	284	12.102	6.419	12.399	1.00	10.74	A	C
ATOM	2110	CD2	LEU	A	284	14.425	7.107	12.953	1.00	10.79	A	C
ATOM	2111	C	LEU	A	284	12.741	10.568	15.245	1.00	10.24	A	C
ATOM	2112	O	LEU	A	284	13.591	11.414	15.013	1.00	9.64	A	O
ATOM	2113	N	LYS	A	285	11.527	10.868	15.682	1.00	10.77	A	N
ATOM	2114	CA	LYS	A	285	11.054	12.217	15.890	1.00	10.81	A	C

ATOM	2115	CB	LYS	A	285	9.544	12.188	16.152	1.00	10.59	A	C
ATOM	2116	CG	LYS	A	285	8.909	13.531	16.527	1.00	10.18	A	C
ATOM	2117	CD	LYS	A	285	7.372	13.380	16.583	1.00	12.54	A	C
ATOM	2118	CE	LYS	A	285	6.660	14.630	17.085	1.00	11.16	A	C
ATOM	2119	NZ	LYS	A	285	5.159	14.525	16.941	1.00	9.27	A	N
ATOM	2120	C	LYS	A	285	11.816	12.886	17.037	1.00	10.86	A	C
ATOM	2121	O	LYS	A	285	12.287	13.995	16.888	1.00	11.16	A	O
ATOM	2122	N	ALA	A	286	11.964	12.194	18.156	1.00	10.94	A	N
ATOM	2123	CA	ALA	A	286	12.744	12.722	19.280	1.00	11.16	A	C
ATOM	2124	CB	ALA	A	286	12.657	11.813	20.437	1.00	11.37	A	C
ATOM	2125	C	ALA	A	286	14.206	12.952	18.897	1.00	10.98	A	C
ATOM	2126	O	ALA	A	286	14.794	13.947	19.275	1.00	10.07	A	O
ATOM	2127	N	ALA	A	287	14.778	12.048	18.115	1.00	11.61	A	N
ATOM	2128	CA	ALA	A	287	16.175	12.206	17.679	1.00	12.13	A	C
ATOM	2129	CB	ALA	A	287	16.692	10.922	17.034	1.00	11.58	A	C
ATOM	2130	C	ALA	A	287	16.349	13.411	16.742	1.00	12.42	A	C
ATOM	2131	O	ALA	A	287	17.310	14.165	16.873	1.00	11.82	A	O
ATOM	2132	N	LEU	A	288	15.407	13.623	15.826	1.00	12.37	A	N
ATOM	2133	CA	LEU	A	288	15.473	14.808	14.956	1.00	13.09	A	C
ATOM	2134	CB	LEU	A	288	14.357	14.775	13.917	1.00	13.67	A	C
ATOM	2135	CG	LEU	A	288	14.552	13.833	12.736	1.00	15.39	A	C
ATOM	2136	CD1	LEU	A	288	13.379	14.033	11.840	1.00	19.44	A	C
ATOM	2137	CD2	LEU	A	288	15.842	14.113	11.974	1.00	15.17	A	C
ATOM	2138	C	LEU	A	288	15.329	16.105	15.747	1.00	12.69	A	C
ATOM	2139	O	LEU	A	288	16.014	17.107	15.481	1.00	12.69	A	O
ATOM	2140	N	ILE	A	289	14.412	16.096	16.704	1.00	12.33	A	N
ATOM	2141	CA	ILE	A	289	14.195	17.261	17.546	1.00	12.69	A	C
ATOM	2142	CB	ILE	A	289	12.920	17.084	18.397	1.00	12.55	A	C
ATOM	2143	CG1	ILE	A	289	11.688	17.178	17.488	1.00	11.46	A	C
ATOM	2144	CD1	ILE	A	289	10.404	16.725	18.104	1.00	10.00	A	C
ATOM	2145	CG2	ILE	A	289	12.869	18.098	19.506	1.00	13.54	A	C
ATOM	2146	C	ILE	A	289	15.412	17.596	18.426	1.00	12.74	A	C
ATOM	2147	O	ILE	A	289	15.844	18.746	18.442	1.00	13.36	A	O
ATOM	2148	N	ALA	A	290	15.975	16.612	19.132	1.00	11.71	A	N
ATOM	2149	CA	ALA	A	290	17.132	16.854	19.976	1.00	11.73	A	C
ATOM	2150	CB	ALA	A	290	17.529	15.593	20.698	1.00	12.08	A	C
ATOM	2151	C	ALA	A	290	18.326	17.370	19.191	1.00	11.95	A	C
ATOM	2152	O	ALA	A	290	19.114	18.198	19.689	1.00	10.65	A	O
ATOM	2153	N	GLY	A	291	18.472	16.866	17.979	1.00	11.84	A	N
ATOM	2154	CA	GLY	A	291	19.633	17.207	17.171	1.00	12.60	A	C
ATOM	2155	C	GLY	A	291	19.466	18.506	16.400	1.00	12.44	A	C
ATOM	2156	O	GLY	A	291	20.437	19.018	15.847	1.00	11.56	A	O
ATOM	2157	N	ALA	A	292	18.249	19.056	16.378	1.00	12.96	A	N
ATOM	2158	CA	ALA	A	292	17.960	20.238	15.562	1.00	13.11	A	C
ATOM	2159	CB	ALA	A	292	16.454	20.468	15.434	1.00	12.99	A	C
ATOM	2160	C	ALA	A	292	18.655	21.499	16.075	1.00	13.45	A	C
ATOM	2161	O	ALA	A	292	18.954	21.612	17.252	1.00	13.95	A	O
ATOM	2162	N	ALA	A	293	18.848	22.456	15.173	1.00	13.18	A	N
ATOM	2163	CA	ALA	A	293	19.567	23.694	15.450	1.00	13.43	A	C
ATOM	2164	CB	ALA	A	293	20.508	24.012	14.284	1.00	13.22	A	C
ATOM	2165	C	ALA	A	293	18.611	24.866	15.637	1.00	13.54	A	C
ATOM	2166	O	ALA	A	293	17.739	25.107	14.812	1.00	13.39	A	O
ATOM	2167	N	ASP	A	294	18.838	25.626	16.691	1.00	13.60	A	N
ATOM	2168	CA	ASP	A	294	18.167	26.895	16.899	1.00	14.04	A	C
ATOM	2169	CB	ASP	A	294	18.590	27.428	18.270	1.00	14.33	A	C
ATOM	2170	CG	ASP	A	294	17.918	28.728	18.634	1.00	14.83	A	C
ATOM	2171	OD1	ASP	A	294	18.142	29.160	19.799	1.00	11.77	A	O
ATOM	2172	OD2	ASP	A	294	17.144	29.360	17.861	1.00	10.92	A	O

ATOM	2173	C	ASP	A	294	18.620	27.814	15.774	1.00	13.72	A	C
ATOM	2174	O	ASP	A	294	19.801	28.075	15.636	1.00	14.66	A	O
ATOM	2175	N	VAL	A	295	17.696	28.304	14.956	1.00	14.43	A	N
ATOM	2176	CA	VAL	A	295	18.057	29.217	13.853	1.00	14.05	A	C
ATOM	2177	CB	VAL	A	295	16.957	29.283	12.730	1.00	13.77	A	C
ATOM	2178	CG1	VAL	A	295	16.670	27.907	12.184	1.00	13.93	A	C
ATOM	2179	CG2	VAL	A	295	15.680	29.956	13.255	1.00	12.53	A	C
ATOM	2180	C	VAL	A	295	18.352	30.622	14.346	1.00	14.82	A	C
ATOM	2181	O	VAL	A	295	18.707	31.497	13.558	1.00	15.77	A	O
ATOM	2182	N	GLY	A	296	18.190	30.857	15.646	1.00	14.99	A	N
ATOM	2183	CA	GLY	A	296	18.450	32.159	16.208	1.00	15.10	A	C
ATOM	2184	C	GLY	A	296	17.282	32.821	16.906	1.00	15.03	A	C
ATOM	2185	O	GLY	A	296	17.458	33.886	17.489	1.00	15.00	A	O
ATOM	2186	N	LEU	A	297	16.114	32.180	16.887	1.00	16.05	A	N
ATOM	2187	CA	LEU	A	297	14.903	32.728	17.501	1.00	15.21	A	C
ATOM	2188	CB	LEU	A	297	13.704	32.420	16.605	1.00	14.95	A	C
ATOM	2189	CG	LEU	A	297	13.881	32.962	15.179	1.00	17.47	A	C
ATOM	2190	CD1	LEU	A	297	12.718	32.507	14.330	1.00	19.73	A	C
ATOM	2191	CD2	LEU	A	297	13.939	34.500	15.204	1.00	18.75	A	C
ATOM	2192	C	LEU	A	297	14.645	32.187	18.903	1.00	15.26	A	C
ATOM	2193	O	LEU	A	297	13.782	32.682	19.636	1.00	14.95	A	O
ATOM	2194	N	GLY	A	298	15.380	31.152	19.266	1.00	15.28	A	N
ATOM	2195	CA	GLY	A	298	15.251	30.546	20.570	1.00	15.27	A	C
ATOM	2196	C	GLY	A	298	14.024	29.691	20.721	1.00	15.55	A	C
ATOM	2197	O	GLY	A	298	13.173	29.572	19.817	1.00	15.07	A	O
ATOM	2198	N	PHE	A	299	13.941	29.090	21.894	1.00	15.47	A	N
ATOM	2199	CA	PHE	A	299	12.820	28.269	22.266	1.00	16.76	A	C
ATOM	2200	CB	PHE	A	299	13.279	26.818	22.539	1.00	16.33	A	C
ATOM	2201	CG	PHE	A	299	14.108	26.237	21.435	1.00	16.07	A	C
ATOM	2202	CD1	PHE	A	299	13.572	26.047	20.167	1.00	15.70	A	C
ATOM	2203	CE1	PHE	A	299	14.349	25.544	19.132	1.00	15.95	A	C
ATOM	2204	CZ	PHE	A	299	15.660	25.233	19.357	1.00	15.27	A	C
ATOM	2205	CE2	PHE	A	299	16.217	25.432	20.610	1.00	15.20	A	C
ATOM	2206	CD2	PHE	A	299	15.436	25.929	21.642	1.00	17.28	A	C
ATOM	2207	C	PHE	A	299	12.200	28.872	23.504	1.00	17.91	A	C
ATOM	2208	O	PHE	A	299	12.886	29.548	24.280	1.00	19.79	A	O
ATOM	2209	N	PRO	A	300	10.904	28.683	23.680	1.00	19.34	A	N
ATOM	2210	CA	PRO	A	300	10.054	27.945	22.747	1.00	20.29	A	C
ATOM	2211	CB	PRO	A	300	8.819	27.671	23.583	1.00	20.94	A	C
ATOM	2212	CG	PRO	A	300	8.712	28.898	24.513	1.00	19.43	A	C
ATOM	2213	CD	PRO	A	300	10.120	29.311	24.758	1.00	20.25	A	C
ATOM	2214	C	PRO	A	300	9.672	28.834	21.581	1.00	20.84	A	C
ATOM	2215	O	PRO	A	300	9.921	30.043	21.655	1.00	21.44	A	O
ATOM	2216	N	ASN	A	301	9.076	28.282	20.524	1.00	21.28	A	N
ATOM	2217	CA	ASN	A	301	8.874	29.078	19.319	1.00	21.53	A	C
ATOM	2218	CB	ASN	A	301	10.198	29.173	18.567	1.00	21.34	A	C
ATOM	2219	CG	ASN	A	301	10.320	30.458	17.764	1.00	20.14	A	C
ATOM	2220	OD1	ASN	A	301	9.875	30.553	16.607	1.00	17.42	A	O
ATOM	2221	ND2	ASN	A	301	10.920	31.454	18.371	1.00	22.84	A	N
ATOM	2222	C	ASN	A	301	7.823	28.534	18.355	1.00	22.14	A	C
ATOM	2223	O	ASN	A	301	7.868	27.379	17.978	1.00	23.49	A	O
ATOM	2224	N	GLY	A	302	6.970	29.416	17.854	1.00	22.24	A	N
ATOM	2225	CA	GLY	A	302	5.912	29.031	16.932	1.00	21.65	A	C
ATOM	2226	C	GLY	A	302	6.292	29.165	15.475	1.00	20.83	A	C
ATOM	2227	O	GLY	A	302	5.574	28.669	14.603	1.00	21.22	A	O
ATOM	2228	N	ASN	A	303	7.446	29.787	15.225	1.00	19.62	A	N
ATOM	2229	CA	ASN	A	303	7.981	30.005	13.886	1.00	17.66	A	C
ATOM	2230	CB	ASN	A	303	8.705	31.349	13.816	1.00	17.45	A	C

ATOM	2231	CG	ASN	A	303	7.872	32.473	14.381	1.00	20.84	A	C
ATOM	2232	OD1	ASN	A	303	6.802	32.779	13.847	1.00	21.34	A	O
ATOM	2233	ND2	ASN	A	303	8.305	33.033	15.530	1.00	22.58	A	N
ATOM	2234	C	ASN	A	303	8.926	28.922	13.414	1.00	15.61	A	C
ATOM	2235	O	ASN	A	303	8.831	28.481	12.239	1.00	13.70	A	O
ATOM	2236	N	GLN	A	304	9.841	28.506	14.298	1.00	14.18	A	N
ATOM	2237	CA	GLN	A	304	10.855	27.513	13.946	1.00	13.13	A	C
ATOM	2238	CB	GLN	A	304	12.235	28.005	14.316	1.00	13.28	A	C
ATOM	2239	CG	GLN	A	304	12.556	27.976	15.811	1.00	12.80	A	C
ATOM	2240	CD	GLN	A	304	14.020	28.087	16.123	1.00	11.63	A	C
ATOM	2241	OE1	GLN	A	304	14.842	27.582	15.386	1.00	13.19	A	O
ATOM	2242	NE2	GLN	A	304	14.352	28.794	17.223	1.00	9.76	A	N
ATOM	2243	C	GLN	A	304	10.601	26.128	14.582	1.00	13.52	A	C
ATOM	2244	O	GLN	A	304	11.372	25.208	14.381	1.00	13.66	A	O
ATOM	2245	N	GLY	A	305	9.537	25.972	15.343	1.00	12.81	A	N
ATOM	2246	CA	GLY	A	305	9.351	24.745	16.101	1.00	12.54	A	C
ATOM	2247	C	GLY	A	305	10.578	24.498	16.970	1.00	12.99	A	C
ATOM	2248	O	GLY	A	305	11.062	25.409	17.633	1.00	11.36	A	O
ATOM	2249	N	TRP	A	306	11.107	23.272	16.926	1.00	12.12	A	N
ATOM	2250	CA	TRP	A	306	12.286	22.898	17.701	1.00	12.07	A	C
ATOM	2251	CB	TRP	A	306	12.130	21.473	18.254	1.00	12.05	A	C
ATOM	2252	CG	TRP	A	306	10.866	21.349	19.092	1.00	11.34	A	C
ATOM	2253	CD1	TRP	A	306	9.755	20.611	18.805	1.00	12.28	A	C
ATOM	2254	NE1	TRP	A	306	8.812	20.766	19.794	1.00	13.42	A	N
ATOM	2255	CE2	TRP	A	306	9.316	21.592	20.761	1.00	12.23	A	C
ATOM	2256	CD2	TRP	A	306	10.616	21.963	20.359	1.00	13.78	A	C
ATOM	2257	CE3	TRP	A	306	11.344	22.822	21.183	1.00	13.41	A	C
ATOM	2258	CZ3	TRP	A	306	10.780	23.247	22.365	1.00	12.96	A	C
ATOM	2259	CH2	TRP	A	306	9.488	22.854	22.735	1.00	13.70	A	C
ATOM	2260	CZ2	TRP	A	306	8.744	22.035	21.945	1.00	14.65	A	C
ATOM	2261	C	TRP	A	306	13.562	23.046	16.890	1.00	12.73	A	C
ATOM	2262	O	TRP	A	306	14.632	22.620	17.318	1.00	14.46	A	O
ATOM	2263	N	GLY	A	307	13.479	23.716	15.741	1.00	13.10	A	N
ATOM	2264	CA	GLY	A	307	14.679	24.111	15.015	1.00	12.18	A	C
ATOM	2265	C	GLY	A	307	14.871	23.392	13.685	1.00	11.91	A	C
ATOM	2266	O	GLY	A	307	14.008	22.628	13.238	1.00	11.20	A	O
ATOM	2267	N	ARG	A	308	16.007	23.658	13.046	1.00	11.60	A	N
ATOM	2268	CA	ARG	A	308	16.299	23.167	11.701	1.00	12.01	A	C
ATOM	2269	CB	ARG	A	308	17.153	24.223	10.961	1.00	12.63	A	C
ATOM	2270	CG	ARG	A	308	17.388	23.970	9.462	1.00	13.43	A	C
ATOM	2271	CD	ARG	A	308	18.284	25.025	8.807	1.00	13.61	A	C
ATOM	2272	NE	ARG	A	308	19.563	25.031	9.510	1.00	16.45	A	N
ATOM	2273	CZ	ARG	A	308	20.127	26.086	10.086	1.00	16.43	A	C
ATOM	2274	NH1	ARG	A	308	21.257	25.902	10.762	1.00	14.45	A	N
ATOM	2275	NH2	ARG	A	308	19.660	27.319	9.902	1.00	13.23	A	N
ATOM	2276	C	ARG	A	308	17.055	21.837	11.770	1.00	12.38	A	C
ATOM	2277	O	ARG	A	308	18.094	21.742	12.434	1.00	12.82	A	O
ATOM	2278	N	VAL	A	309	16.549	20.817	11.080	1.00	11.99	A	N
ATOM	2279	CA	VAL	A	309	17.170	19.498	11.096	1.00	12.04	A	C
ATOM	2280	CB	VAL	A	309	16.553	18.573	10.051	1.00	11.35	A	C
ATOM	2281	CG1	VAL	A	309	17.354	17.272	9.961	1.00	11.45	A	C
ATOM	2282	CG2	VAL	A	309	15.047	18.335	10.377	1.00	11.38	A	C
ATOM	2283	C	VAL	A	309	18.667	19.545	10.868	1.00	12.28	A	C
ATOM	2284	O	VAL	A	309	19.148	20.157	9.930	1.00	11.94	A	O
ATOM	2285	N	THR	A	310	19.393	18.904	11.760	1.00	13.11	A	N
ATOM	2286	CA	THR	A	310	20.854	18.814	11.675	1.00	12.86	A	C
ATOM	2287	CB	THR	A	310	21.471	19.719	12.723	1.00	13.26	A	C
ATOM	2288	OG1	THR	A	310	21.044	21.090	12.516	1.00	12.98	A	O



ATOM	2289	CG2	THR	A	310	22.962	19.747	12.610	1.00	13.68	A	C
ATOM	2290	C	THR	A	310	21.197	17.347	11.911	1.00	13.94	A	C
ATOM	2291	O	THR	A	310	21.411	16.896	13.064	1.00	14.93	A	O
ATOM	2292	N	LEU	A	311	21.269	16.601	10.818	1.00	13.28	A	N
ATOM	2293	CA	LEU	A	311	21.110	15.149	10.879	1.00	14.11	A	C
ATOM	2294	CB	LEU	A	311	20.956	14.589	9.463	1.00	13.67	A	C
ATOM	2295	CG	LEU	A	311	20.879	13.078	9.311	1.00	13.50	A	C
ATOM	2296	CD1	LEU	A	311	19.749	12.522	10.109	1.00	15.11	A	C
ATOM	2297	CD2	LEU	A	311	20.749	12.688	7.849	1.00	14.22	A	C
ATOM	2298	C	LEU	A	311	22.252	14.455	11.605	1.00	14.58	A	C
ATOM	2299	O	LEU	A	311	22.012	13.521	12.345	1.00	14.74	A	O
ATOM	2300	N	ASP	A	312	23.483	14.959	11.462	1.00	15.58	A	N
ATOM	2301	CA	ASP	A	312	24.624	14.307	12.111	1.00	16.68	A	C
ATOM	2302	CB	ASP	A	312	25.984	14.797	11.582	1.00	16.93	A	C
ATOM	2303	CG	ASP	A	312	26.222	16.245	11.822	1.00	19.05	A	C
ATOM	2304	OD1	ASP	A	312	27.394	16.614	11.755	1.00	25.94	A	O
ATOM	2305	OD2	ASP	A	312	25.348	17.090	12.090	1.00	18.31	A	O
ATOM	2306	C	ASP	A	312	24.560	14.330	13.615	1.00	16.48	A	C
ATOM	2307	O	ASP	A	312	24.965	13.381	14.241	1.00	17.40	A	O
ATOM	2308	N	LYS	A	313	23.976	15.364	14.202	1.00	16.32	A	N
ATOM	2309	CA	LYS	A	313	23.755	15.366	15.641	1.00	16.35	A	C
ATOM	2310	CB	LYS	A	313	23.363	16.773	16.130	1.00	17.66	A	C
ATOM	2311	CG	LYS	A	313	24.430	17.848	15.938	1.00	20.65	A	C
ATOM	2312	CD	LYS	A	313	24.735	18.590	17.250	1.00	28.29	A	C
ATOM	2313	CE	LYS	A	313	25.619	17.746	18.162	1.00	31.10	A	C
ATOM	2314	NZ	LYS	A	313	26.458	18.529	19.131	1.00	32.31	A	N
ATOM	2315	C	LYS	A	313	22.666	14.379	16.100	1.00	15.36	A	C
ATOM	2316	O	LYS	A	313	22.662	13.968	17.258	1.00	15.49	A	O
ATOM	2317	N	SER	A	314	21.755	14.007	15.212	1.00	14.12	A	N
ATOM	2318	CA	SER	A	314	20.700	13.047	15.537	1.00	13.37	A	C
ATOM	2319	CB	SER	A	314	19.497	13.217	14.590	1.00	13.56	A	C
ATOM	2320	OG	SER	A	314	18.889	14.489	14.723	1.00	11.16	A	O
ATOM	2321	C	SER	A	314	21.148	11.581	15.505	1.00	14.53	A	C
ATOM	2322	O	SER	A	314	20.507	10.717	16.112	1.00	14.30	A	O
ATOM	2323	N	LEU	A	315	22.209	11.285	14.771	1.00	14.58	A	N
ATOM	2324	CA	LEU	A	315	22.563	9.896	14.484	1.00	15.64	A	C
ATOM	2325	CB	LEU	A	315	23.750	9.824	13.505	1.00	15.15	A	C
ATOM	2326	CG	LEU	A	315	23.506	10.436	12.143	1.00	14.88	A	C
ATOM	2327	CD1	LEU	A	315	24.834	10.445	11.360	1.00	16.67	A	C
ATOM	2328	CD2	LEU	A	315	22.401	9.683	11.411	1.00	16.28	A	C
ATOM	2329	C	LEU	A	315	22.905	9.095	15.733	1.00	16.16	A	C
ATOM	2330	O	LEU	A	315	22.442	7.956	15.894	1.00	16.79	A	O
ATOM	2331	N	ASN	A	316	23.692	9.686	16.631	1.00	17.60	A	N
ATOM	2332	CA	ASN	A	316	24.235	8.915	17.749	1.00	17.99	A	C
ATOM	2333	CB	ASN	A	316	25.757	8.837	17.694	1.00	19.59	A	C
ATOM	2334	CG	ASN	A	316	26.264	7.879	16.601	1.00	22.56	A	C
ATOM	2335	OD1	ASN	A	316	25.736	6.732	16.397	1.00	21.64	A	O
ATOM	2336	ND2	ASN	A	316	27.321	8.320	15.910	1.00	23.13	A	N
ATOM	2337	C	ASN	A	316	23.732	9.396	19.116	1.00	17.61	A	C
ATOM	2338	O	ASN	A	316	24.390	9.212	20.152	1.00	15.93	A	O
ATOM	2339	N	VAL	A	317	22.505	9.912	19.123	1.00	15.75	A	N
ATOM	2340	CA	VAL	A	317	21.820	10.220	20.389	1.00	15.40	A	C
ATOM	2341	CB	VAL	A	317	20.360	10.675	20.150	1.00	15.21	A	C
ATOM	2342	CG1	VAL	A	317	20.335	11.940	19.350	1.00	16.28	A	C
ATOM	2343	CG2	VAL	A	317	19.547	9.600	19.458	1.00	16.07	A	C
ATOM	2344	C	VAL	A	317	21.803	8.995	21.323	1.00	14.67	A	C
ATOM	2345	O	VAL	A	317	21.675	7.864	20.868	1.00	14.77	A	O
ATOM	2346	N	ALA	A	318	21.932	9.225	22.627	1.00	13.95	A	N



ATOM	2347	CA	ALA	A	318	21.623	8.186	23.603	1.00	13.64	A	C
ATOM	2348	CB	ALA	A	318	22.196	8.523	24.940	1.00	13.50	A	C
ATOM	2349	C	ALA	A	318	20.087	8.130	23.652	1.00	13.19	A	C
ATOM	2350	O	ALA	A	318	19.416	9.168	23.498	1.00	13.46	A	O
ATOM	2351	N	PHE	A	319	19.512	6.952	23.853	1.00	12.88	A	N
ATOM	2352	CA	PHE	A	319	18.076	6.824	23.633	1.00	12.66	A	C
ATOM	2353	CB	PHE	A	319	17.815	6.531	22.137	1.00	12.79	A	C
ATOM	2354	CG	PHE	A	319	18.267	5.158	21.700	1.00	14.03	A	C
ATOM	2355	CD1	PHE	A	319	19.504	4.980	21.107	1.00	12.44	A	C
ATOM	2356	CE1	PHE	A	319	19.930	3.725	20.718	1.00	15.58	A	C
ATOM	2357	CZ	PHE	A	319	19.115	2.619	20.921	1.00	15.26	A	C
ATOM	2358	CE2	PHE	A	319	17.887	2.777	21.524	1.00	14.77	A	C
ATOM	2359	CD2	PHE	A	319	17.461	4.047	21.905	1.00	15.05	A	C
ATOM	2360	C	PHE	A	319	17.349	5.799	24.461	1.00	12.38	A	C
ATOM	2361	O	PHE	A	319	17.947	4.918	25.055	1.00	12.11	A	O
ATOM	2362	N	VAL	A	320	16.032	5.947	24.488	1.00	12.04	A	N
ATOM	2363	CA	VAL	A	320	15.125	4.909	24.949	1.00	12.42	A	C
ATOM	2364	CB	VAL	A	320	14.391	5.323	26.252	1.00	13.15	A	C
ATOM	2365	CG1	VAL	A	320	13.237	4.331	26.589	1.00	13.46	A	C
ATOM	2366	CG2	VAL	A	320	15.401	5.395	27.416	1.00	13.91	A	C
ATOM	2367	C	VAL	A	320	14.137	4.758	23.802	1.00	11.88	A	C
ATOM	2368	O	VAL	A	320	13.668	5.749	23.271	1.00	10.13	A	O
ATOM	2369	N	ASN	A	321	13.824	3.520	23.441	1.00	11.82	A	N
ATOM	2370	CA	ASN	A	321	13.018	3.205	22.261	1.00	11.75	A	C
ATOM	2371	CB	ASN	A	321	13.858	2.323	21.313	1.00	11.75	A	C
ATOM	2372	CG	ASN	A	321	13.214	2.117	19.944	1.00	12.10	A	C
ATOM	2373	OD1	ASN	A	321	12.506	3.005	19.437	1.00	12.86	A	O
ATOM	2374	ND2	ASN	A	321	13.451	0.919	19.328	1.00	10.43	A	N
ATOM	2375	C	ASN	A	321	11.711	2.463	22.637	1.00	12.63	A	C
ATOM	2376	O	ASN	A	321	11.509	1.311	22.260	1.00	12.41	A	O
ATOM	2377	N	GLU	A	322	10.835	3.130	23.380	1.00	12.99	A	N
ATOM	2378	CA	GLU	A	322	9.542	2.552	23.760	1.00	13.23	A	C
ATOM	2379	CB	GLU	A	322	8.601	2.415	22.528	1.00	13.10	A	C
ATOM	2380	CG	GLU	A	322	8.146	3.794	22.013	1.00	12.18	A	C
ATOM	2381	CD	GLU	A	322	7.072	3.781	20.933	1.00	14.48	A	C
ATOM	2382	OE1	GLU	A	322	6.747	4.884	20.429	1.00	15.20	A	O
ATOM	2383	OE2	GLU	A	322	6.564	2.690	20.588	1.00	14.00	A	O
ATOM	2384	C	GLU	A	322	9.654	1.239	24.556	1.00	14.04	A	C
ATOM	2385	O	GLU	A	322	8.778	0.385	24.468	1.00	12.70	A	O
ATOM	2386	N	THR	A	323	10.688	1.122	25.387	1.00	13.33	A	N
ATOM	2387	CA	THR	A	323	10.907	-0.101	26.145	1.00	14.72	A	C
ATOM	2388	CB	THR	A	323	12.375	-0.466	26.173	1.00	14.45	A	C
ATOM	2389	OG1	THR	A	323	13.168	0.721	26.401	1.00	16.74	A	O
ATOM	2390	CG2	THR	A	323	12.813	-0.980	24.810	1.00	15.39	A	C
ATOM	2391	C	THR	A	323	10.397	-0.045	27.589	1.00	15.63	A	C
ATOM	2392	O	THR	A	323	10.572	-1.011	28.319	1.00	14.71	A	O
ATOM	2393	N	SER	A	324	9.796	1.073	28.002	1.00	15.41	A	N
ATOM	2394	CA	SER	A	324	9.176	1.159	29.341	1.00	15.78	A	C
ATOM	2395	CB	SER	A	324	10.008	2.045	30.272	1.00	15.94	A	C
ATOM	2396	OG	SER	A	324	11.281	1.460	30.594	1.00	17.86	A	O
ATOM	2397	C	SER	A	324	7.739	1.723	29.257	1.00	15.74	A	C
ATOM	2398	O	SER	A	324	7.558	2.937	29.315	1.00	15.93	A	O
ATOM	2399	N	PRO	A	325	6.729	0.864	29.118	1.00	16.08	A	N
ATOM	2400	CA	PRO	A	325	5.326	1.306	29.170	1.00	17.17	A	C
ATOM	2401	CB	PRO	A	325	4.525	0.035	28.823	1.00	17.76	A	C
ATOM	2402	CG	PRO	A	325	5.454	-1.106	29.084	1.00	17.45	A	C
ATOM	2403	CD	PRO	A	325	6.845	-0.585	28.885	1.00	16.38	A	C
ATOM	2404	C	PRO	A	325	4.926	1.815	30.548	1.00	17.68	A	C

ATOM	2405	O	PRO	A	325	5.277	1.211	31.553	1.00	18.68	A	O
ATOM	2406	N	LEU	A	326	4.204	2.916	30.596	1.00	18.30	A	N
ATOM	2407	CA	LEU	A	326	3.796	3.491	31.871	1.00	18.53	A	C
ATOM	2408	CB	LEU	A	326	4.410	4.890	32.059	1.00	18.37	A	C
ATOM	2409	CG	LEU	A	326	5.938	5.027	32.161	1.00	19.30	A	C
ATOM	2410	CD1	LEU	A	326	6.350	6.502	32.200	1.00	20.03	A	C
ATOM	2411	CD2	LEU	A	326	6.471	4.338	33.387	1.00	17.55	A	C
ATOM	2412	C	LEU	A	326	2.287	3.605	31.982	1.00	19.08	A	C
ATOM	2413	O	LEU	A	326	1.589	3.926	30.989	1.00	18.42	A	O
ATOM	2414	N	SER	A	327	1.810	3.326	33.201	1.00	19.13	A	N
ATOM	2415	CA	SER	A	327	0.438	3.607	33.672	1.00	19.58	A	C
ATOM	2416	CB	SER	A	327	-0.123	2.391	34.397	1.00	19.04	A	C
ATOM	2417	OG	SER	A	327	-0.176	1.357	33.434	1.00	19.38	A	O
ATOM	2418	C	SER	A	327	0.558	4.902	34.476	1.00	19.58	A	C
ATOM	2419	O	SER	A	327	1.609	5.154	35.075	1.00	18.88	A	O
ATOM	2420	N	THR	A	328	-0.505	5.696	34.595	1.00	20.38	A	N
ATOM	2421	CA	THR	A	328	-0.861	6.454	35.789	1.00	19.96	A	C
ATOM	2422	CB	THR	A	328	-2.343	6.678	35.951	1.00	20.43	A	C
ATOM	2423	OG1	THR	A	328	-2.870	7.047	34.681	1.00	20.32	A	O
ATOM	2424	CG2	THR	A	328	-2.602	7.922	36.842	1.00	21.84	A	C
ATOM	2425	C	THR	A	328	-0.102	6.262	37.084	1.00	19.51	A	C
ATOM	2426	O	THR	A	328	-0.223	5.222	37.739	1.00	19.59	A	O
ATOM	2427	N	SER	A	329	0.732	7.268	37.356	1.00	18.40	A	N
ATOM	2428	CA	SER	A	329	1.489	7.464	38.588	1.00	19.19	A	C
ATOM	2429	CB	BSER	A	329	0.679	7.017	39.818	0.50	19.34	A	C
ATOM	2430	CB	ASER	A	329	0.629	7.141	39.833	0.50	19.52	A	C
ATOM	2431	OG	BSER	A	329	0.653	5.599	39.887	0.50	18.73	A	O
ATOM	2432	OG	ASER	A	329	-0.672	7.722	39.718	0.50	20.52	A	O
ATOM	2433	C	SER	A	329	2.792	6.686	38.588	1.00	18.71	A	C
ATOM	2434	O	SER	A	329	3.533	6.753	39.550	1.00	18.11	A	O
ATOM	2435	N	GLN	A	330	3.066	5.936	37.524	1.00	17.70	A	N
ATOM	2436	CA	GLN	A	330	4.339	5.250	37.420	1.00	17.71	A	C
ATOM	2437	CB	GLN	A	330	4.193	4.001	36.566	1.00	17.37	A	C
ATOM	2438	CG	GLN	A	330	3.233	2.970	37.168	1.00	17.60	A	C
ATOM	2439	CD	GLN	A	330	3.116	1.700	36.319	1.00	18.11	A	C
ATOM	2440	OE1	GLN	A	330	3.305	1.763	35.119	1.00	16.08	A	O
ATOM	2441	NE2	GLN	A	330	2.762	0.550	36.952	1.00	15.56	A	N
ATOM	2442	C	GLN	A	330	5.401	6.195	36.837	1.00	18.14	A	C
ATOM	2443	O	GLN	A	330	5.103	7.308	36.423	1.00	18.07	A	O
ATOM	2444	N	LYS	A	331	6.643	5.750	36.842	1.00	18.66	A	N
ATOM	2445	CA	LYS	A	331	7.710	6.524	36.276	1.00	19.23	A	C
ATOM	2446	CB	LYS	A	331	8.229	7.550	37.289	1.00	20.19	A	C
ATOM	2447	CG	LYS	A	331	8.972	6.934	38.450	1.00	23.65	A	C
ATOM	2448	CD	LYS	A	331	9.071	7.912	39.625	1.00	28.70	A	C
ATOM	2449	CE	LYS	A	331	9.954	7.332	40.754	1.00	31.64	A	C
ATOM	2450	NZ	LYS	A	331	10.409	8.388	41.729	1.00	34.93	A	N
ATOM	2451	C	LYS	A	331	8.804	5.589	35.820	1.00	18.87	A	C
ATOM	2452	O	LYS	A	331	8.887	4.410	36.261	1.00	18.18	A	O
ATOM	2453	N	ALA	A	332	9.587	6.091	34.873	1.00	17.37	A	N
ATOM	2454	CA	ALA	A	332	10.797	5.406	34.412	1.00	17.82	A	C
ATOM	2455	CB	ALA	A	332	10.689	5.068	32.941	1.00	17.06	A	C
ATOM	2456	C	ALA	A	332	11.991	6.324	34.650	1.00	17.33	A	C
ATOM	2457	O	ALA	A	332	11.999	7.480	34.213	1.00	16.52	A	O
ATOM	2458	N	THR	A	333	13.005	5.805	35.325	1.00	17.85	A	N
ATOM	2459	CA	THR	A	333	14.108	6.643	35.784	1.00	17.61	A	C
ATOM	2460	CB	THR	A	333	14.194	6.544	37.304	1.00	18.03	A	C
ATOM	2461	OG1	THR	A	333	12.956	6.966	37.902	1.00	19.93	A	O
ATOM	2462	CG2	THR	A	333	15.234	7.490	37.851	1.00	18.18	A	C

ATOM	2463	C	THR	A	333	15.410	6.186	35.159	1.00	17.36	A	C
ATOM	2464	O	THR	A	333	15.727	4.987	35.162	1.00	17.40	A	O
ATOM	2465	N	TYR	A	334	16.176	7.135	34.628	1.00	17.05	A	N
ATOM	2466	CA	TYR	A	334	17.437	6.840	33.986	1.00	17.42	A	C
ATOM	2467	CB	TYR	A	334	17.308	6.975	32.464	1.00	16.94	A	C
ATOM	2468	CG	TYR	A	334	16.144	6.230	31.860	1.00	16.41	A	C
ATOM	2469	CD1	TYR	A	334	16.273	4.891	31.458	1.00	14.43	A	C
ATOM	2470	CE1	TYR	A	334	15.205	4.205	30.912	1.00	14.63	A	C
ATOM	2471	CZ	TYR	A	334	13.977	4.846	30.772	1.00	15.02	A	C
ATOM	2472	OH	TYR	A	334	12.929	4.188	30.216	1.00	16.23	A	O
ATOM	2473	CE2	TYR	A	334	13.819	6.147	31.153	1.00	15.62	A	C
ATOM	2474	CD2	TYR	A	334	14.907	6.835	31.718	1.00	16.76	A	C
ATOM	2475	C	TYR	A	334	18.542	7.767	34.455	1.00	17.66	A	C
ATOM	2476	O	TYR	A	334	18.279	8.840	34.991	1.00	16.79	A	O
ATOM	2477	N	SER	A	335	19.783	7.375	34.169	1.00	17.44	A	N
ATOM	2478	CA	SER	A	335	20.939	8.218	34.442	1.00	18.62	A	C
ATOM	2479	CB	BSER	A	335	21.879	7.537	35.433	0.50	18.54	A	C
ATOM	2480	CB	ASER	A	335	21.916	7.518	35.393	0.50	18.59	A	C
ATOM	2481	OG	BSER	A	335	22.697	6.585	34.783	0.50	18.97	A	O
ATOM	2482	OG	ASER	A	335	21.316	7.174	36.629	0.50	19.43	A	O
ATOM	2483	C	SER	A	335	21.680	8.538	33.128	1.00	18.52	A	C
ATOM	2484	O	SER	A	335	21.698	7.720	32.221	1.00	18.14	A	O
ATOM	2485	N	PHE	A	336	22.298	9.715	33.049	1.00	17.92	A	N
ATOM	2486	CA	PHE	A	336	23.115	10.092	31.911	1.00	18.36	A	C
ATOM	2487	CB	PHE	A	336	22.324	10.949	30.900	1.00	18.52	A	C
ATOM	2488	CG	PHE	A	336	23.150	11.401	29.753	1.00	17.47	A	C
ATOM	2489	CD1	PHE	A	336	23.733	12.667	29.739	1.00	18.88	A	C
ATOM	2490	CE1	PHE	A	336	24.529	13.067	28.654	1.00	18.14	A	C
ATOM	2491	CZ	PHE	A	336	24.749	12.198	27.591	1.00	18.35	A	C
ATOM	2492	CE2	PHE	A	336	24.174	10.936	27.601	1.00	18.49	A	C
ATOM	2493	CD2	PHE	A	336	23.386	10.543	28.681	1.00	19.03	A	C
ATOM	2494	C	PHE	A	336	24.314	10.898	32.403	1.00	18.74	A	C
ATOM	2495	O	PHE	A	336	24.159	11.810	33.195	1.00	18.98	A	O
ATOM	2496	N	THR	A	337	25.504	10.547	31.938	1.00	19.28	A	N
ATOM	2497	CA	THR	A	337	26.733	11.219	32.364	1.00	19.77	A	C
ATOM	2498	CB	THR	A	337	27.879	10.201	32.343	1.00	20.11	A	C
ATOM	2499	OG1	THR	A	337	27.609	9.175	33.321	1.00	19.75	A	O
ATOM	2500	CG2	THR	A	337	29.159	10.857	32.796	1.00	21.58	A	C
ATOM	2501	C	THR	A	337	27.096	12.369	31.440	1.00	20.14	A	C
ATOM	2502	O	THR	A	337	27.266	12.163	30.253	1.00	20.10	A	O
ATOM	2503	N	ALA	A	338	27.181	13.571	32.000	1.00	19.74	A	N
ATOM	2504	CA	ALA	A	338	27.487	14.793	31.259	1.00	20.23	A	C
ATOM	2505	CB	ALA	A	338	26.468	15.858	31.588	1.00	19.43	A	C
ATOM	2506	C	ALA	A	338	28.881	15.292	31.633	1.00	20.94	A	C
ATOM	2507	O	ALA	A	338	29.389	14.991	32.710	1.00	19.43	A	O
ATOM	2508	N	GLN	A	339	29.503	16.042	30.741	1.00	22.51	A	N
ATOM	2509	CA	GLN	A	339	30.750	16.711	31.070	1.00	23.12	A	C
ATOM	2510	CB	GLN	A	339	31.893	16.162	30.230	1.00	24.34	A	C
ATOM	2511	CG	GLN	A	339	32.591	14.904	30.726	1.00	29.11	A	C
ATOM	2512	CD	GLN	A	339	34.116	14.923	30.437	1.00	36.99	A	C
ATOM	2513	OE1	GLN	A	339	34.841	13.991	30.825	1.00	41.39	A	O
ATOM	2514	NE2	GLN	A	339	34.597	15.995	29.778	1.00	36.90	A	N
ATOM	2515	C	GLN	A	339	30.543	18.167	30.722	1.00	23.27	A	C
ATOM	2516	O	GLN	A	339	30.034	18.485	29.641	1.00	23.02	A	O
ATOM	2517	N	ALA	A	340	30.922	19.061	31.619	1.00	22.60	A	N
ATOM	2518	CA	ALA	A	340	30.793	20.492	31.347	1.00	22.71	A	C
ATOM	2519	CB	ALA	A	340	31.311	21.296	32.535	1.00	22.84	A	C
ATOM	2520	C	ALA	A	340	31.524	20.916	30.076	1.00	22.30	A	C

ATOM	2521	O	ALA	A	340	32.474	20.270	29.650	1.00	22.44	A	O
ATOM	2522	N	GLY	A	341	31.063	21.996	29.455	1.00	23.38	A	N
ATOM	2523	CA	GLY	A	341	31.738	22.554	28.283	1.00	23.73	A	C
ATOM	2524	C	GLY	A	341	30.989	22.425	26.956	1.00	24.15	A	C
ATOM	2525	O	GLY	A	341	31.457	22.902	25.917	1.00	24.10	A	O
ATOM	2526	N	LYS	A	342	29.829	21.774	26.970	1.00	24.05	A	N
ATOM	2527	CA	LYS	A	342	29.038	21.637	25.743	1.00	24.39	A	C
ATOM	2528	CB	LYS	A	342	29.643	20.545	24.861	1.00	25.08	A	C
ATOM	2529	CG	LYS	A	342	29.610	19.148	25.496	1.00	27.13	A	C
ATOM	2530	CD	LYS	A	342	30.471	18.173	24.723	1.00	29.40	A	C
ATOM	2531	CE	LYS	A	342	30.254	16.725	25.182	1.00	29.96	A	C
ATOM	2532	NZ	LYS	A	342	30.738	16.515	26.576	1.00	32.09	A	N
ATOM	2533	C	LYS	A	342	27.552	21.373	26.058	1.00	23.40	A	C
ATOM	2534	O	LYS	A	342	27.220	20.861	27.144	1.00	23.54	A	O
ATOM	2535	N	PRO	A	343	26.652	21.755	25.151	1.00	22.09	A	N
ATOM	2536	CA	PRO	A	343	25.219	21.683	25.450	1.00	21.01	A	C
ATOM	2537	CB	PRO	A	343	24.557	22.206	24.163	1.00	21.58	A	C
ATOM	2538	CG	PRO	A	343	25.613	23.026	23.492	1.00	22.06	A	C
ATOM	2539	CD	PRO	A	343	26.902	22.348	23.820	1.00	22.30	A	C
ATOM	2540	C	PRO	A	343	24.729	20.279	25.756	1.00	19.35	A	C
ATOM	2541	O	PRO	A	343	25.311	19.298	25.317	1.00	17.82	A	O
ATOM	2542	N	LEU	A	344	23.645	20.223	26.521	1.00	18.12	A	N
ATOM	2543	CA	LEU	A	344	22.945	18.988	26.790	1.00	17.07	A	C
ATOM	2544	CB	LEU	A	344	23.019	18.680	28.278	1.00	17.12	A	C
ATOM	2545	CG	LEU	A	344	22.250	17.476	28.788	1.00	16.96	A	C
ATOM	2546	CD1	LEU	A	344	22.743	16.188	28.128	1.00	16.29	A	C
ATOM	2547	CD2	LEU	A	344	22.399	17.414	30.336	1.00	17.28	A	C
ATOM	2548	C	LEU	A	344	21.484	19.168	26.360	1.00	16.41	A	C
ATOM	2549	O	LEU	A	344	20.814	20.029	26.870	1.00	17.49	A	O
ATOM	2550	N	LYS	A	345	21.013	18.336	25.440	1.00	15.23	A	N
ATOM	2551	CA	LYS	A	345	19.638	18.405	24.943	1.00	14.51	A	C
ATOM	2552	CB	LYS	A	345	19.644	18.807	23.474	1.00	14.84	A	C
ATOM	2553	CG	LYS	A	345	20.104	20.235	23.248	1.00	13.82	A	C
ATOM	2554	CD	LYS	A	345	19.987	20.664	21.795	1.00	16.32	A	C
ATOM	2555	CE	LYS	A	345	18.599	21.126	21.423	1.00	13.96	A	C
ATOM	2556	NZ	LYS	A	345	18.513	21.491	19.992	1.00	17.70	A	N
ATOM	2557	C	LYS	A	345	18.929	17.066	25.135	1.00	14.25	A	C
ATOM	2558	O	LYS	A	345	19.399	16.033	24.658	1.00	14.33	A	O
ATOM	2559	N	ILE	A	346	17.821	17.084	25.870	1.00	13.41	A	N
ATOM	2560	CA	ILE	A	346	17.031	15.888	26.116	1.00	13.30	A	C
ATOM	2561	CB	ILE	A	346	16.983	15.589	27.619	1.00	13.25	A	C
ATOM	2562	CG1	ILE	A	346	18.376	15.444	28.197	1.00	13.74	A	C
ATOM	2563	CD1	ILE	A	346	18.459	15.807	29.637	1.00	15.75	A	C
ATOM	2564	CG2	ILE	A	346	16.180	14.329	27.874	1.00	13.54	A	C
ATOM	2565	C	ILE	A	346	15.598	16.084	25.601	1.00	13.26	A	C
ATOM	2566	O	ILE	A	346	14.900	17.010	26.020	1.00	13.15	A	O
ATOM	2567	N	SER	A	347	15.159	15.197	24.714	1.00	12.65	A	N
ATOM	2568	CA	SER	A	347	13.795	15.262	24.172	1.00	12.47	A	C
ATOM	2569	CB	BSER	A	347	13.838	15.473	22.654	0.35	12.36	A	C
ATOM	2570	CB	ASER	A	347	13.813	15.524	22.662	0.65	12.73	A	C
ATOM	2571	OG	BSER	A	347	12.569	15.297	22.042	0.35	10.59	A	O
ATOM	2572	OG	ASER	A	347	14.655	16.634	22.329	0.65	13.18	A	O
ATOM	2573	C	SER	A	347	13.032	13.983	24.491	1.00	11.72	A	C
ATOM	2574	O	SER	A	347	13.511	12.881	24.219	1.00	11.81	A	O
ATOM	2575	N	LEU	A	348	11.830	14.165	25.026	1.00	11.03	A	N
ATOM	2576	CA	LEU	A	348	10.864	13.121	25.289	1.00	10.93	A	C
ATOM	2577	CB	LEU	A	348	10.302	13.274	26.706	1.00	10.96	A	C
ATOM	2578	CG	LEU	A	348	9.054	12.502	27.097	1.00	10.80	A	C



ATOM	2579	CD1	LEU	A	348	9.396	11.029	27.180	1.00	13.05	A	C
ATOM	2580	CD2	LEU	A	348	8.542	12.969	28.443	1.00	12.50	A	C
ATOM	2581	C	LEU	A	348	9.735	13.231	24.287	1.00	11.09	A	C
ATOM	2582	O	LEU	A	348	9.152	14.302	24.140	1.00	12.01	A	O
ATOM	2583	N	VAL	A	349	9.389	12.127	23.631	1.00	10.58	A	N
ATOM	2584	CA	VAL	A	349	8.327	12.142	22.638	1.00	11.32	A	C
ATOM	2585	CB	VAL	A	349	8.876	12.223	21.185	1.00	11.27	A	C
ATOM	2586	CG1	VAL	A	349	7.745	12.102	20.169	1.00	12.19	A	C
ATOM	2587	CG2	VAL	A	349	9.653	13.511	20.961	1.00	11.93	A	C
ATOM	2588	C	VAL	A	349	7.522	10.873	22.768	1.00	11.68	A	C
ATOM	2589	O	VAL	A	349	8.099	9.802	22.870	1.00	12.43	A	O
ATOM	2590	N	TRP	A	350	6.200	10.993	22.768	1.00	11.69	A	N
ATOM	2591	CA	TRP	A	350	5.354	9.813	22.662	1.00	11.48	A	C
ATOM	2592	CB	TRP	A	350	4.719	9.442	24.002	1.00	11.79	A	C
ATOM	2593	CG	TRP	A	350	3.822	10.448	24.628	1.00	11.11	A	C
ATOM	2594	CD1	TRP	A	350	2.457	10.378	24.720	1.00	12.11	A	C
ATOM	2595	NE1	TRP	A	350	1.961	11.469	25.386	1.00	12.24	A	N
ATOM	2596	CE2	TRP	A	350	3.015	12.262	25.774	1.00	13.16	A	C
ATOM	2597	CD2	TRP	A	350	4.208	11.640	25.311	1.00	13.33	A	C
ATOM	2598	CE3	TRP	A	350	5.440	12.249	25.593	1.00	12.51	A	C
ATOM	2599	CZ3	TRP	A	350	5.444	13.449	26.311	1.00	13.31	A	C
ATOM	2600	CH2	TRP	A	350	4.248	14.022	26.767	1.00	13.75	A	C
ATOM	2601	CZ2	TRP	A	350	3.022	13.427	26.507	1.00	13.59	A	C
ATOM	2602	C	TRP	A	350	4.314	9.883	21.536	1.00	11.50	A	C
ATOM	2603	O	TRP	A	350	3.905	10.953	21.077	1.00	11.90	A	O
ATOM	2604	N	SER	A	351	3.921	8.707	21.071	1.00	11.83	A	N
ATOM	2605	CA	SER	A	351	2.889	8.607	20.070	1.00	12.20	A	C
ATOM	2606	CB	SER	A	351	3.182	7.496	19.070	1.00	12.11	A	C
ATOM	2607	OG	SER	A	351	4.356	7.772	18.310	1.00	11.85	A	O
ATOM	2608	C	SER	A	351	1.636	8.378	20.884	1.00	12.65	A	C
ATOM	2609	O	SER	A	351	1.360	7.285	21.375	1.00	12.72	A	O
ATOM	2610	N	ASP	A	352	0.947	9.477	21.115	1.00	13.75	A	N
ATOM	2611	CA	ASP	A	352	-0.205	9.532	21.982	1.00	14.48	A	C
ATOM	2612	CB	ASP	A	352	-0.508	11.003	22.225	1.00	14.84	A	C
ATOM	2613	CG	ASP	A	352	-1.480	11.251	23.385	1.00	16.70	A	C
ATOM	2614	OD1	ASP	A	352	-1.655	10.366	24.260	1.00	15.50	A	O
ATOM	2615	OD2	ASP	A	352	-2.115	12.329	23.458	1.00	15.19	A	O
ATOM	2616	C	ASP	A	352	-1.427	8.842	21.389	1.00	15.19	A	C
ATOM	2617	O	ASP	A	352	-1.569	8.678	20.155	1.00	15.52	A	O
ATOM	2618	N	ALA	A	353	-2.331	8.434	22.273	1.00	15.26	A	N
ATOM	2619	CA	ALA	A	353	-3.689	8.074	21.853	1.00	15.65	A	C
ATOM	2620	CB	ALA	A	353	-4.526	7.801	23.051	1.00	15.59	A	C
ATOM	2621	C	ALA	A	353	-4.325	9.197	21.018	1.00	15.42	A	C
ATOM	2622	O	ALA	A	353	-4.076	10.374	21.264	1.00	15.11	A	O
ATOM	2623	N	PRO	A	354	-5.157	8.840	20.041	1.00	16.50	A	N
ATOM	2624	CA	PRO	A	354	-5.858	9.841	19.235	1.00	16.92	A	C
ATOM	2625	CB	PRO	A	354	-6.724	9.003	18.287	1.00	17.36	A	C
ATOM	2626	CG	PRO	A	354	-6.790	7.646	18.897	1.00	17.45	A	C
ATOM	2627	CD	PRO	A	354	-5.499	7.456	19.640	1.00	16.81	A	C
ATOM	2628	C	PRO	A	354	-6.723	10.771	20.073	1.00	18.05	A	C
ATOM	2629	O	PRO	A	354	-7.420	10.293	20.957	1.00	17.51	A	O
ATOM	2630	N	GLY	A	355	-6.629	12.074	19.819	1.00	18.60	A	N
ATOM	2631	CA	GLY	A	355	-7.392	13.071	20.527	1.00	20.06	A	C
ATOM	2632	C	GLY	A	355	-8.773	13.285	19.936	1.00	21.21	A	C
ATOM	2633	O	GLY	A	355	-9.095	12.758	18.880	1.00	22.41	A	O
ATOM	2634	N	SER	A	356	-9.598	14.050	20.628	1.00	22.87	A	N
ATOM	2635	CA	SER	A	356	-10.939	14.377	20.145	1.00	23.97	A	C
ATOM	2636	CB	SER	A	356	-11.924	14.555	21.319	1.00	24.97	A	C



ATOM	2637	OG	SER	A	356	-12.771	15.696	21.117	1.00	26.85	A	O
ATOM	2638	C	SER	A	356	-10.901	15.654	19.320	1.00	24.04	A	C
ATOM	2639	O	SER	A	356	-10.151	16.583	19.635	1.00	23.54	A	O
ATOM	2640	N	THR	A	357	-11.714	15.684	18.261	1.00	24.61	A	N
ATOM	2641	CA	THR	A	357	-11.826	16.846	17.396	1.00	25.58	A	C
ATOM	2642	CB	THR	A	357	-12.423	16.436	16.032	1.00	25.86	A	C
ATOM	2643	OG1	THR	A	357	-13.673	15.748	16.218	1.00	25.91	A	O
ATOM	2644	CG2	THR	A	357	-11.534	15.392	15.334	1.00	25.30	A	C
ATOM	2645	C	THR	A	357	-12.687	17.982	18.000	1.00	26.58	A	C
ATOM	2646	O	THR	A	357	-12.812	19.035	17.398	1.00	26.22	A	O
ATOM	2647	N	THR	A	358	-13.276	17.771	19.175	1.00	27.59	A	N
ATOM	2648	CA	THR	A	358	-14.113	18.816	19.779	1.00	28.37	A	C
ATOM	2649	CB	THR	A	358	-15.575	18.335	19.938	1.00	28.27	A	C
ATOM	2650	OG1	THR	A	358	-15.606	17.065	20.606	1.00	28.60	A	O
ATOM	2651	CG2	THR	A	358	-16.192	18.066	18.587	1.00	27.97	A	C
ATOM	2652	C	THR	A	358	-13.605	19.321	21.118	1.00	28.71	A	C
ATOM	2653	O	THR	A	358	-13.954	20.424	21.524	1.00	29.22	A	O
ATOM	2654	N	ALA	A	359	-12.758	18.548	21.795	1.00	28.63	A	N
ATOM	2655	CA	ALA	A	359	-12.311	18.925	23.133	1.00	27.94	A	C
ATOM	2656	CB	ALA	A	359	-11.668	17.739	23.814	1.00	28.64	A	C
ATOM	2657	C	ALA	A	359	-11.349	20.100	23.099	1.00	27.98	A	C
ATOM	2658	O	ALA	A	359	-10.738	20.393	22.060	1.00	27.61	A	O
ATOM	2659	N	SER	A	360	-11.213	20.785	24.241	1.00	27.18	A	N
ATOM	2660	CA	SER	A	360	-10.301	21.916	24.344	1.00	27.00	A	C
ATOM	2661	CB	SER	A	360	-10.351	22.564	25.737	1.00	27.57	A	C
ATOM	2662	OG	SER	A	360	-11.688	22.840	26.125	1.00	31.54	A	O
ATOM	2663	C	SER	A	360	-8.858	21.485	24.060	1.00	25.14	A	C
ATOM	2664	O	SER	A	360	-8.115	22.230	23.446	1.00	24.27	A	O
ATOM	2665	N	LEU	A	361	-8.478	20.307	24.553	1.00	23.74	A	N
ATOM	2666	CA	LEU	A	361	-7.100	19.812	24.453	1.00	23.54	A	C
ATOM	2667	CB	LEU	A	361	-6.480	19.583	25.840	1.00	23.87	A	C
ATOM	2668	CG	LEU	A	361	-6.119	20.802	26.702	1.00	27.30	A	C
ATOM	2669	CD1	LEU	A	361	-5.434	20.335	27.980	1.00	28.61	A	C
ATOM	2670	CD2	LEU	A	361	-5.217	21.827	25.975	1.00	28.84	A	C
ATOM	2671	C	LEU	A	361	-7.097	18.493	23.701	1.00	21.78	A	C
ATOM	2672	O	LEU	A	361	-7.942	17.611	23.961	1.00	21.73	A	O
ATOM	2673	N	THR	A	362	-6.141	18.325	22.790	1.00	19.81	A	N
ATOM	2674	CA	THR	A	362	-6.053	17.058	22.066	1.00	18.76	A	C
ATOM	2675	CB	THR	A	362	-5.433	17.230	20.657	1.00	19.42	A	C
ATOM	2676	OG1	THR	A	362	-4.100	17.707	20.786	1.00	17.51	A	O
ATOM	2677	CG2	THR	A	362	-6.174	18.305	19.862	1.00	20.58	A	C
ATOM	2678	C	THR	A	362	-5.261	16.023	22.819	1.00	17.21	A	C
ATOM	2679	O	THR	A	362	-5.411	14.858	22.530	1.00	13.79	A	O
ATOM	2680	N	LEU	A	363	-4.398	16.448	23.761	1.00	16.68	A	N
ATOM	2681	CA	LEU	A	363	-3.560	15.505	24.484	1.00	16.39	A	C
ATOM	2682	CB	LEU	A	363	-2.547	16.213	25.411	1.00	16.30	A	C
ATOM	2683	CG	LEU	A	363	-1.460	15.318	25.990	1.00	16.62	A	C
ATOM	2684	CD1	LEU	A	363	-0.380	14.960	24.939	1.00	16.31	A	C
ATOM	2685	CD2	LEU	A	363	-0.838	15.936	27.236	1.00	15.84	A	C
ATOM	2686	C	LEU	A	363	-4.424	14.536	25.280	1.00	17.11	A	C
ATOM	2687	O	LEU	A	363	-5.404	14.936	25.911	1.00	17.15	A	O
ATOM	2688	N	VAL	A	364	-4.068	13.253	25.249	1.00	16.50	A	N
ATOM	2689	CA	VAL	A	364	-4.829	12.263	25.975	1.00	16.09	A	C
ATOM	2690	CB	VAL	A	364	-5.285	11.121	25.030	1.00	15.79	A	C
ATOM	2691	CG1	VAL	A	364	-5.871	9.933	25.826	1.00	17.24	A	C
ATOM	2692	CG2	VAL	A	364	-6.288	11.651	24.020	1.00	16.26	A	C
ATOM	2693	C	VAL	A	364	-3.983	11.744	27.139	1.00	15.68	A	C
ATOM	2694	O	VAL	A	364	-4.329	11.942	28.309	1.00	15.17	A	O

ATOM	2695	N	ASN	A	365	-2.875	11.085	26.809	1.00	14.41	A	N
ATOM	2696	CA	ASN	A	365	-1.931	10.614	27.804	1.00	14.31	A	C
ATOM	2697	CB	ASN	A	365	-1.302	9.286	27.354	1.00	14.31	A	C
ATOM	2698	CG	ASN	A	365	-2.342	8.161	27.214	1.00	16.21	A	C
ATOM	2699	OD1	ASN	A	365	-3.298	8.081	28.004	1.00	13.31	A	O
ATOM	2700	ND2	ASN	A	365	-2.158	7.283	26.206	1.00	14.49	A	N
ATOM	2701	C	ASN	A	365	-0.858	11.690	28.088	1.00	14.80	A	C
ATOM	2702	O	ASN	A	365	-0.174	12.190	27.172	1.00	14.01	A	O
ATOM	2703	N	ASP	A	366	-0.696	12.015	29.360	1.00	14.06	A	N
ATOM	2704	CA	ASP	A	366	0.158	13.115	29.783	1.00	15.00	A	C
ATOM	2705	CB	ASP	A	366	-0.632	14.068	30.672	1.00	14.40	A	C
ATOM	2706	CG	ASP	A	366	0.105	15.346	30.990	1.00	15.13	A	C
ATOM	2707	OD1	ASP	A	366	1.344	15.467	30.710	1.00	13.15	A	O
ATOM	2708	OD2	ASP	A	366	-0.491	16.284	31.609	1.00	17.79	A	O
ATOM	2709	C	ASP	A	366	1.367	12.568	30.548	1.00	14.89	A	C
ATOM	2710	O	ASP	A	366	1.257	12.132	31.708	1.00	15.57	A	O
ATOM	2711	N	LEU	A	367	2.501	12.562	29.865	1.00	14.16	A	N
ATOM	2712	CA	LEU	A	367	3.772	12.248	30.462	1.00	14.65	A	C
ATOM	2713	CB	LEU	A	367	4.581	11.333	29.520	1.00	14.37	A	C
ATOM	2714	CG	LEU	A	367	3.990	10.005	29.077	1.00	13.06	A	C
ATOM	2715	CD1	LEU	A	367	5.063	9.220	28.244	1.00	12.20	A	C
ATOM	2716	CD2	LEU	A	367	3.485	9.123	30.239	1.00	15.25	A	C
ATOM	2717	C	LEU	A	367	4.523	13.555	30.710	1.00	14.15	A	C
ATOM	2718	O	LEU	A	367	4.271	14.546	30.045	1.00	14.17	A	O
ATOM	2719	N	ASP	A	368	5.441	13.556	31.677	1.00	14.04	A	N
ATOM	2720	CA	ASP	A	368	6.271	14.705	31.980	1.00	14.28	A	C
ATOM	2721	CB	ASP	A	368	5.959	15.284	33.354	1.00	15.52	A	C
ATOM	2722	CG	ASP	A	368	4.529	15.726	33.515	1.00	17.54	A	C
ATOM	2723	OD1	ASP	A	368	3.909	16.253	32.540	1.00	14.48	A	O
ATOM	2724	OD2	ASP	A	368	4.006	15.624	34.642	1.00	17.39	A	O
ATOM	2725	C	ASP	A	368	7.724	14.275	32.057	1.00	14.49	A	C
ATOM	2726	O	ASP	A	368	8.034	13.203	32.587	1.00	13.94	A	O
ATOM	2727	N	LEU	A	369	8.603	15.108	31.520	1.00	14.32	A	N
ATOM	2728	CA	LEU	A	369	10.044	14.937	31.645	1.00	14.31	A	C
ATOM	2729	CB	LEU	A	369	10.735	15.448	30.380	1.00	13.72	A	C
ATOM	2730	CG	LEU	A	369	12.238	15.284	30.298	1.00	12.96	A	C
ATOM	2731	CD1	LEU	A	369	12.572	13.850	30.345	1.00	12.52	A	C
ATOM	2732	CD2	LEU	A	369	12.749	15.953	28.980	1.00	14.11	A	C
ATOM	2733	C	LEU	A	369	10.539	15.733	32.854	1.00	15.02	A	C
ATOM	2734	O	LEU	A	369	10.218	16.922	33.012	1.00	15.50	A	O
ATOM	2735	N	VAL	A	370	11.315	15.085	33.698	1.00	15.26	A	N
ATOM	2736	CA	VAL	A	370	11.875	15.729	34.905	1.00	15.63	A	C
ATOM	2737	CB	VAL	A	370	11.144	15.278	36.180	1.00	15.95	A	C
ATOM	2738	CG1	VAL	A	370	11.679	16.020	37.425	1.00	17.73	A	C
ATOM	2739	CG2	VAL	A	370	9.687	15.487	36.024	1.00	15.57	A	C
ATOM	2740	C	VAL	A	370	13.359	15.388	34.975	1.00	15.46	A	C
ATOM	2741	O	VAL	A	370	13.767	14.219	35.042	1.00	15.96	A	O
ATOM	2742	N	ILE	A	371	14.174	16.422	34.908	1.00	15.15	A	N
ATOM	2743	CA	ILE	A	371	15.608	16.261	34.858	1.00	14.98	A	C
ATOM	2744	CB	ILE	A	371	16.171	17.036	33.669	1.00	14.71	A	C
ATOM	2745	CG1	ILE	A	371	15.509	16.589	32.336	1.00	14.63	A	C
ATOM	2746	CD1	ILE	A	371	15.600	15.075	32.072	1.00	14.66	A	C
ATOM	2747	CG2	ILE	A	371	17.674	16.922	33.614	1.00	12.85	A	C
ATOM	2748	C	ILE	A	371	16.145	16.835	36.155	1.00	15.95	A	C
ATOM	2749	O	ILE	A	371	15.648	17.853	36.618	1.00	16.74	A	O
ATOM	2750	N	THR	A	372	17.150	16.174	36.727	1.00	16.86	A	N
ATOM	2751	CA	THR	A	372	17.858	16.671	37.897	1.00	17.19	A	C
ATOM	2752	CB	THR	A	372	17.618	15.748	39.089	1.00	17.36	A	C

ATOM	2753	OG1	THR	A	372	16.212	15.514	39.265	1.00	18.17	A	O
ATOM	2754	CG2	THR	A	372	18.044	16.409	40.372	1.00	17.84	A	C
ATOM	2755	C	THR	A	372	19.364	16.729	37.634	1.00	17.65	A	C
ATOM	2756	O	THR	A	372	19.962	15.725	37.262	1.00	18.44	A	O
ATOM	2757	N	ALA	A	373	19.971	17.891	37.870	1.00	17.80	A	N
ATOM	2758	CA	ALA	A	373	21.376	18.118	37.606	1.00	18.13	A	C
ATOM	2759	CB	ALA	A	373	21.643	19.607	37.475	1.00	18.43	A	C
ATOM	2760	C	ALA	A	373	22.175	17.545	38.767	1.00	19.16	A	C
ATOM	2761	O	ALA	A	373	21.601	17.188	39.780	1.00	18.57	A	O
ATOM	2762	N	PRO	A	374	23.479	17.368	38.581	1.00	19.84	A	N
ATOM	2763	CA	PRO	A	374	24.348	16.857	39.642	1.00	20.99	A	C
ATOM	2764	CB	PRO	A	374	25.727	16.884	39.001	1.00	20.60	A	C
ATOM	2765	CG	PRO	A	374	25.434	16.700	37.530	1.00	20.96	A	C
ATOM	2766	CD	PRO	A	374	24.174	17.460	37.286	1.00	20.29	A	C
ATOM	2767	C	PRO	A	374	24.266	17.647	40.948	1.00	22.06	A	C
ATOM	2768	O	PRO	A	374	24.303	17.039	42.011	1.00	23.95	A	O
ATOM	2769	N	ASN	A	375	24.024	18.954	40.873	1.00	23.03	A	N
ATOM	2770	CA	ASN	A	375	23.910	19.770	42.058	1.00	23.32	A	C
ATOM	2771	CB	ASN	A	375	24.515	21.165	41.790	1.00	24.03	A	C
ATOM	2772	CG	ASN	A	375	23.581	22.096	40.993	1.00	26.93	A	C
ATOM	2773	OD1	ASN	A	375	22.515	21.689	40.492	1.00	28.51	A	O
ATOM	2774	ND2	ASN	A	375	23.987	23.362	40.878	1.00	27.28	A	N
ATOM	2775	C	ASN	A	375	22.471	19.898	42.563	1.00	23.07	A	C
ATOM	2776	O	ASN	A	375	22.208	20.711	43.430	1.00	22.92	A	O
ATOM	2777	N	GLY	A	376	21.541	19.120	42.010	1.00	21.76	A	N
ATOM	2778	CA	GLY	A	376	20.166	19.165	42.469	1.00	21.43	A	C
ATOM	2779	C	GLY	A	376	19.197	20.077	41.724	1.00	20.91	A	C
ATOM	2780	O	GLY	A	376	17.990	20.006	41.937	1.00	19.94	A	O
ATOM	2781	N	THR	A	377	19.696	20.909	40.828	1.00	21.29	A	N
ATOM	2782	CA	THR	A	377	18.793	21.785	40.090	1.00	21.36	A	C
ATOM	2783	CB	THR	A	377	19.571	22.738	39.220	1.00	21.19	A	C
ATOM	2784	OG1	THR	A	377	20.423	23.532	40.054	1.00	22.26	A	O
ATOM	2785	CG2	THR	A	377	18.635	23.724	38.538	1.00	20.97	A	C
ATOM	2786	C	THR	A	377	17.818	20.971	39.239	1.00	20.56	A	C
ATOM	2787	O	THR	A	377	18.206	20.058	38.541	1.00	19.93	A	O
ATOM	2788	N	LYS	A	378	16.558	21.345	39.315	1.00	20.68	A	N
ATOM	2789	CA	LYS	A	378	15.488	20.630	38.644	1.00	21.64	A	C
ATOM	2790	CB	LYS	A	378	14.321	20.503	39.594	1.00	22.42	A	C
ATOM	2791	CG	LYS	A	378	13.709	19.168	39.611	1.00	28.13	A	C
ATOM	2792	CD	LYS	A	378	14.144	18.449	40.913	1.00	33.32	A	C
ATOM	2793	CE	LYS	A	378	13.743	17.001	40.854	1.00	34.92	A	C
ATOM	2794	NZ	LYS	A	378	14.605	16.111	41.699	1.00	38.61	A	N
ATOM	2795	C	LYS	A	378	14.990	21.344	37.397	1.00	20.06	A	C
ATOM	2796	O	LYS	A	378	14.902	22.553	37.388	1.00	19.59	A	O
ATOM	2797	N	TYR	A	379	14.623	20.568	36.378	1.00	18.59	A	N
ATOM	2798	CA	TYR	A	379	14.009	21.088	35.155	1.00	17.87	A	C
ATOM	2799	CB	TYR	A	379	15.030	21.111	34.011	1.00	17.25	A	C
ATOM	2800	CG	TYR	A	379	16.382	21.654	34.386	1.00	17.53	A	C
ATOM	2801	CD1	TYR	A	379	17.297	20.864	35.052	1.00	18.58	A	C
ATOM	2802	CE1	TYR	A	379	18.537	21.352	35.417	1.00	19.05	A	C
ATOM	2803	CZ	TYR	A	379	18.895	22.655	35.097	1.00	21.25	A	C
ATOM	2804	OH	TYR	A	379	20.160	23.104	35.465	1.00	20.46	A	O
ATOM	2805	CE2	TYR	A	379	18.004	23.459	34.399	1.00	19.58	A	C
ATOM	2806	CD2	TYR	A	379	16.751	22.953	34.060	1.00	18.07	A	C
ATOM	2807	C	TYR	A	379	12.852	20.198	34.732	1.00	17.42	A	C
ATOM	2808	O	TYR	A	379	12.967	18.973	34.766	1.00	18.13	A	O
ATOM	2809	N	VAL	A	380	11.732	20.787	34.340	1.00	16.44	A	N
ATOM	2810	CA	VAL	A	380	10.653	19.989	33.750	1.00	16.11	A	C

ATOM	2811	CB	VAL	A	380	9.320	20.114	34.514	1.00	16.66	A	C
ATOM	2812	CG1	VAL	A	380	9.521	19.742	36.000	1.00	17.64	A	C
ATOM	2813	CG2	VAL	A	380	8.716	21.505	34.369	1.00	16.52	A	C
ATOM	2814	C	VAL	A	380	10.466	20.353	32.283	1.00	14.93	A	C
ATOM	2815	O	VAL	A	380	10.876	21.425	31.826	1.00	15.17	A	O
ATOM	2816	N	GLY	A	381	9.868	19.436	31.547	1.00	14.19	A	N
ATOM	2817	CA	GLY	A	381	9.761	19.541	30.101	1.00	13.85	A	C
ATOM	2818	C	GLY	A	381	9.132	20.847	29.647	1.00	13.74	A	C
ATOM	2819	O	GLY	A	381	8.096	21.259	30.153	1.00	13.57	A	O
ATOM	2820	N	ASN	A	382	9.813	21.509	28.729	1.00	13.87	A	N
ATOM	2821	CA	ASN	A	382	9.332	22.719	28.064	1.00	14.08	A	C
ATOM	2822	CB	ASN	A	382	8.002	22.451	27.344	1.00	13.91	A	C
ATOM	2823	CG	ASN	A	382	8.148	21.436	26.209	1.00	14.03	A	C
ATOM	2824	OD1	ASN	A	382	9.250	21.181	25.757	1.00	13.23	A	O
ATOM	2825	ND2	ASN	A	382	7.041	20.850	25.770	1.00	10.67	A	N
ATOM	2826	C	ASN	A	382	9.232	23.942	28.966	1.00	14.58	A	C
ATOM	2827	O	ASN	A	382	8.682	24.981	28.556	1.00	14.15	A	O
ATOM	2828	N	ASP	A	383	9.796	23.869	30.178	1.00	14.75	A	N
ATOM	2829	CA	ASP	A	383	9.813	25.057	31.017	1.00	14.97	A	C
ATOM	2830	CB	ASP	A	383	9.593	24.709	32.499	1.00	15.34	A	C
ATOM	2831	CG	ASP	A	383	9.580	25.952	33.388	1.00	15.81	A	C
ATOM	2832	OD1	ASP	A	383	9.786	27.082	32.845	1.00	16.83	A	O
ATOM	2833	OD2	ASP	A	383	9.394	25.897	34.636	1.00	15.84	A	O
ATOM	2834	C	ASP	A	383	11.127	25.813	30.810	1.00	15.13	A	C
ATOM	2835	O	ASP	A	383	12.160	25.490	31.398	1.00	15.46	A	O
ATOM	2836	N	PHE	A	384	11.074	26.859	30.000	1.00	15.11	A	N
ATOM	2837	CA	PHE	A	384	12.284	27.559	29.589	1.00	15.10	A	C
ATOM	2838	CB	PHE	A	384	12.178	27.818	28.086	1.00	16.52	A	C
ATOM	2839	CG	PHE	A	384	12.247	26.560	27.240	1.00	14.23	A	C
ATOM	2840	CD1	PHE	A	384	13.440	25.910	27.059	1.00	19.41	A	C
ATOM	2841	CE1	PHE	A	384	13.516	24.782	26.273	1.00	19.08	A	C
ATOM	2842	CZ	PHE	A	384	12.395	24.303	25.685	1.00	18.05	A	C
ATOM	2843	CE2	PHE	A	384	11.208	24.943	25.845	1.00	14.73	A	C
ATOM	2844	CD2	PHE	A	384	11.140	26.070	26.602	1.00	16.74	A	C
ATOM	2845	C	PHE	A	384	12.546	28.857	30.389	1.00	15.96	A	C
ATOM	2846	O	PHE	A	384	13.547	29.558	30.152	1.00	15.13	A	O
ATOM	2847	N	THR	A	385	11.666	29.151	31.350	1.00	16.18	A	N
ATOM	2848	CA	THR	A	385	11.820	30.294	32.264	1.00	17.37	A	C
ATOM	2849	CB	THR	A	385	10.519	31.097	32.400	1.00	17.19	A	C
ATOM	2850	OG1	THR	A	385	9.520	30.295	33.030	1.00	17.98	A	O
ATOM	2851	CG2	THR	A	385	9.922	31.491	31.028	1.00	18.21	A	C
ATOM	2852	C	THR	A	385	12.238	29.868	33.689	1.00	17.95	A	C
ATOM	2853	O	THR	A	385	11.703	28.890	34.252	1.00	17.41	A	O
ATOM	2854	N	ALA	A	386	13.197	30.599	34.250	1.00	18.54	A	N
ATOM	2855	CA	ALA	A	386	13.743	30.266	35.565	1.00	19.43	A	C
ATOM	2856	CB	ALA	A	386	15.056	30.971	35.792	1.00	19.87	A	C
ATOM	2857	C	ALA	A	386	12.728	30.697	36.594	1.00	20.06	A	C
ATOM	2858	O	ALA	A	386	12.078	31.735	36.409	1.00	21.03	A	O
ATOM	2859	N	PRO	A	387	12.525	29.897	37.635	1.00	19.71	A	N
ATOM	2860	CA	PRO	A	387	13.134	28.582	37.766	1.00	20.17	A	C
ATOM	2861	CB	PRO	A	387	12.951	28.269	39.250	1.00	20.90	A	C
ATOM	2862	CG	PRO	A	387	11.609	28.910	39.587	1.00	20.16	A	C
ATOM	2863	CD	PRO	A	387	11.670	30.223	38.796	1.00	21.11	A	C
ATOM	2864	C	PRO	A	387	12.413	27.549	36.890	1.00	19.33	A	C
ATOM	2865	O	PRO	A	387	11.237	27.688	36.612	1.00	18.07	A	O
ATOM	2866	N	TYR	A	388	13.144	26.521	36.491	1.00	19.24	A	N
ATOM	2867	CA	TYR	A	388	12.781	25.672	35.365	1.00	19.24	A	C
ATOM	2868	CB	TYR	A	388	14.059	25.211	34.661	1.00	18.91	A	C



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ATOM	2869	CG	TYR	A	388	14.912	26.363	34.177	1.00	18.51	A	C
ATOM	2870	CD1	TYR	A	388	16.128	26.625	34.761	1.00	16.61	A	C
ATOM	2871	CE1	TYR	A	388	16.912	27.701	34.350	1.00	17.76	A	C
ATOM	2872	CZ	TYR	A	388	16.462	28.511	33.312	1.00	15.12	A	C
ATOM	2873	OH	TYR	A	388	17.242	29.565	32.918	1.00	17.69	A	O
ATOM	2874	CE2	TYR	A	388	15.241	28.276	32.723	1.00	14.50	A	C
ATOM	2875	CD2	TYR	A	388	14.462	27.229	33.154	1.00	14.33	A	C
ATOM	2876	C	TYR	A	388	11.934	24.467	35.745	1.00	19.73	A	C
ATOM	2877	O	TYR	A	388	11.688	23.598	34.913	1.00	19.79	A	O
ATOM	2878	N	ASP	A	389	11.422	24.442	36.972	1.00	20.38	A	N
ATOM	2879	CA	ASP	A	389	10.605	23.327	37.430	1.00	21.41	A	C
ATOM	2880	CB	ASP	A	389	11.346	22.547	38.507	1.00	22.04	A	C
ATOM	2881	CG	ASP	A	389	11.504	23.343	39.796	1.00	24.83	A	C
ATOM	2882	OD1	ASP	A	389	11.618	22.706	40.869	1.00	27.95	A	O
ATOM	2883	OD2	ASP	A	389	11.523	24.595	39.822	1.00	24.63	A	O
ATOM	2884	C	ASP	A	389	9.246	23.724	37.968	1.00	21.64	A	C
ATOM	2885	O	ASP	A	389	8.629	22.947	38.709	1.00	22.12	A	O
ATOM	2886	N	ASN	A	390	8.759	24.908	37.618	1.00	21.45	A	N
ATOM	2887	CA	ASN	A	390	7.455	25.326	38.130	1.00	22.14	A	C
ATOM	2888	CB	ASN	A	390	7.555	26.664	38.892	1.00	22.91	A	C
ATOM	2889	CG	ASN	A	390	7.965	27.825	37.989	1.00	23.08	A	C
ATOM	2890	OD1	ASN	A	390	8.404	27.620	36.847	1.00	22.98	A	O
ATOM	2891	ND2	ASN	A	390	7.816	29.050	38.491	1.00	23.21	A	N
ATOM	2892	C	ASN	A	390	6.356	25.402	37.060	1.00	22.16	A	C
ATOM	2893	O	ASN	A	390	5.181	25.500	37.405	1.00	21.88	A	O
ATOM	2894	N	ASN	A	391	6.717	25.340	35.772	1.00	21.51	A	N
ATOM	2895	CA	ASN	A	391	5.705	25.411	34.713	1.00	20.98	A	C
ATOM	2896	CB	ASN	A	391	5.986	26.567	33.728	1.00	21.22	A	C
ATOM	2897	CG	ASN	A	391	6.221	27.924	34.426	1.00	22.34	A	C
ATOM	2898	OD1	ASN	A	391	7.345	28.481	34.388	1.00	22.21	A	O
ATOM	2899	ND2	ASN	A	391	5.151	28.490	35.029	1.00	23.08	A	N
ATOM	2900	C	ASN	A	391	5.611	24.072	33.978	1.00	20.79	A	C
ATOM	2901	O	ASN	A	391	6.295	23.818	32.978	1.00	21.08	A	O
ATOM	2902	N	TRP	A	392	4.741	23.211	34.467	1.00	20.10	A	N
ATOM	2903	CA	TRP	A	392	4.601	21.862	33.928	1.00	20.04	A	C
ATOM	2904	CB	TRP	A	392	3.893	20.979	34.926	1.00	20.74	A	C
ATOM	2905	CG	TRP	A	392	4.629	20.757	36.231	1.00	24.30	A	C
ATOM	2906	CD1	TRP	A	392	4.687	21.605	37.309	1.00	28.54	A	C
ATOM	2907	NE1	TRP	A	392	5.435	21.038	38.317	1.00	30.71	A	N
ATOM	2908	CE2	TRP	A	392	5.870	19.804	37.902	1.00	28.29	A	C
ATOM	2909	CD2	TRP	A	392	5.367	19.594	36.598	1.00	27.17	A	C
ATOM	2910	CE3	TRP	A	392	5.695	18.400	35.937	1.00	29.38	A	C
ATOM	2911	CZ3	TRP	A	392	6.456	17.447	36.608	1.00	28.54	A	C
ATOM	2912	CH2	TRP	A	392	6.922	17.683	37.904	1.00	30.49	A	C
ATOM	2913	CZ2	TRP	A	392	6.643	18.857	38.566	1.00	30.31	A	C
ATOM	2914	C	TRP	A	392	3.767	21.890	32.661	1.00	19.03	A	C
ATOM	2915	O	TRP	A	392	2.828	22.678	32.552	1.00	19.40	A	O
ATOM	2916	N	ASP	A	393	4.107	21.020	31.709	1.00	17.66	A	N
ATOM	2917	CA	ASP	A	393	3.416	20.958	30.424	1.00	16.59	A	C
ATOM	2918	CB	ASP	A	393	4.431	20.669	29.332	1.00	16.47	A	C
ATOM	2919	CG	ASP	A	393	3.813	20.660	27.930	1.00	15.80	A	C
ATOM	2920	OD1	ASP	A	393	4.350	21.364	27.045	1.00	14.98	A	O
ATOM	2921	OD2	ASP	A	393	2.817	19.975	27.629	1.00	15.12	A	O
ATOM	2922	C	ASP	A	393	2.324	19.888	30.425	1.00	16.46	A	C
ATOM	2923	O	ASP	A	393	2.606	18.716	30.648	1.00	15.65	A	O
ATOM	2924	N	GLY	A	394	1.080	20.302	30.178	1.00	15.96	A	N
ATOM	2925	CA	GLY	A	394	-0.029	19.384	30.014	1.00	16.13	A	C
ATOM	2926	C	GLY	A	394	-0.747	19.498	28.675	1.00	16.27	A	C



ATOM	2927	O	GLY	A	394	-1.936	19.255	28.601	1.00	16.15	A	O
ATOM	2928	N	ARG	A	395	-0.030	19.864	27.617	1.00	17.31	A	N
ATOM	2929	CA	ARG	A	395	-0.607	19.978	26.264	1.00	17.68	A	C
ATOM	2930	CB	ARG	A	395	-0.588	21.437	25.783	1.00	19.08	A	C
ATOM	2931	CG	ARG	A	395	-1.434	22.408	26.518	1.00	26.02	A	C
ATOM	2932	CD	ARG	A	395	-1.172	23.839	26.066	1.00	31.34	A	C
ATOM	2933	NE	ARG	A	395	-1.802	24.813	26.969	1.00	37.30	A	N
ATOM	2934	CZ	ARG	A	395	-3.026	25.331	26.821	1.00	40.58	A	C
ATOM	2935	NH1	ARG	A	395	-3.478	26.216	27.717	1.00	44.12	A	N
ATOM	2936	NH2	ARG	A	395	-3.805	24.983	25.805	1.00	40.20	A	N
ATOM	2937	C	ARG	A	395	0.176	19.240	25.165	1.00	15.80	A	C
ATOM	2938	O	ARG	A	395	-0.418	18.827	24.176	1.00	16.01	A	O
ATOM	2939	N	ASN	A	396	1.502	19.212	25.282	1.00	14.41	A	N
ATOM	2940	CA	ASN	A	396	2.389	18.645	24.251	1.00	13.89	A	C
ATOM	2941	CB	ASN	A	396	3.662	19.483	24.133	1.00	13.10	A	C
ATOM	2942	CG	ASN	A	396	3.408	20.889	23.585	1.00	14.63	A	C
ATOM	2943	OD1	ASN	A	396	3.129	21.075	22.374	1.00	11.53	A	O
ATOM	2944	ND2	ASN	A	396	3.550	21.897	24.463	1.00	11.89	A	N
ATOM	2945	C	ASN	A	396	2.806	17.197	24.475	1.00	13.64	A	C
ATOM	2946	O	ASN	A	396	2.995	16.743	25.634	1.00	14.92	A	O
ATOM	2947	N	ASN	A	397	2.973	16.452	23.376	1.00	13.56	A	N
ATOM	2948	CA	ASN	A	397	3.539	15.085	23.451	1.00	12.37	A	C
ATOM	2949	CB	ASN	A	397	2.705	14.080	22.672	1.00	12.41	A	C
ATOM	2950	CG	ASN	A	397	2.539	14.450	21.192	1.00	13.07	A	C
ATOM	2951	OD1	ASN	A	397	2.243	15.594	20.849	1.00	12.07	A	O
ATOM	2952	ND2	ASN	A	397	2.683	13.466	20.324	1.00	13.08	A	N
ATOM	2953	C	ASN	A	397	5.011	15.077	23.010	1.00	13.13	A	C
ATOM	2954	O	ASN	A	397	5.607	14.010	22.663	1.00	11.34	A	O
ATOM	2955	N	VAL	A	398	5.577	16.291	23.028	1.00	12.66	A	N
ATOM	2956	CA	VAL	A	398	6.992	16.524	22.914	1.00	12.58	A	C
ATOM	2957	CB	VAL	A	398	7.329	17.261	21.626	1.00	13.06	A	C
ATOM	2958	CG1	VAL	A	398	8.835	17.523	21.533	1.00	11.41	A	C
ATOM	2959	CG2	VAL	A	398	6.846	16.476	20.408	1.00	12.98	A	C
ATOM	2960	C	VAL	A	398	7.381	17.412	24.105	1.00	12.92	A	C
ATOM	2961	O	VAL	A	398	6.819	18.501	24.272	1.00	13.08	A	O
ATOM	2962	N	GLU	A	399	8.288	16.913	24.945	1.00	12.47	A	N
ATOM	2963	CA	GLU	A	399	8.797	17.666	26.107	1.00	12.81	A	C
ATOM	2964	CB	GLU	A	399	8.339	17.054	27.452	1.00	12.40	A	C
ATOM	2965	CG	GLU	A	399	6.870	17.340	27.793	1.00	11.56	A	C
ATOM	2966	CD	GLU	A	399	6.538	17.357	29.284	1.00	13.58	A	C
ATOM	2967	OE1	GLU	A	399	5.312	17.324	29.635	1.00	14.48	A	O
ATOM	2968	OE2	GLU	A	399	7.471	17.421	30.112	1.00	14.20	A	O
ATOM	2969	C	GLU	A	399	10.307	17.680	26.052	1.00	12.44	A	C
ATOM	2970	O	GLU	A	399	10.920	16.624	25.929	1.00	13.16	A	O
ATOM	2971	N	ASN	A	400	10.890	18.883	26.174	1.00	12.69	A	N
ATOM	2972	CA	ASN	A	400	12.326	19.098	26.073	1.00	12.36	A	C
ATOM	2973	CB	ASN	A	400	12.636	19.953	24.822	1.00	12.37	A	C
ATOM	2974	CG	ASN	A	400	12.185	19.302	23.559	1.00	14.26	A	C
ATOM	2975	OD1	ASN	A	400	12.621	18.213	23.247	1.00	16.94	A	O
ATOM	2976	ND2	ASN	A	400	11.302	19.964	22.817	1.00	14.56	A	N
ATOM	2977	C	ASN	A	400	12.959	19.820	27.254	1.00	11.55	A	C
ATOM	2978	O	ASN	A	400	12.363	20.716	27.867	1.00	11.03	A	O
ATOM	2979	N	VAL	A	401	14.200	19.448	27.543	1.00	11.83	A	N
ATOM	2980	CA	VAL	A	401	15.042	20.183	28.494	1.00	11.67	A	C
ATOM	2981	CB	VAL	A	401	15.230	19.394	29.804	1.00	11.24	A	C
ATOM	2982	CG1	VAL	A	401	16.317	20.017	30.668	1.00	13.18	A	C
ATOM	2983	CG2	VAL	A	401	13.962	19.359	30.558	1.00	11.36	A	C
ATOM	2984	C	VAL	A	401	16.351	20.372	27.792	1.00	12.10	A	C

ATOM	2985	O	VAL	A	401	17.022	19.394	27.471	1.00	12.05	A	O
ATOM	2986	N	PHE	A	402	16.693	21.634	27.528	1.00	12.69	A	N
ATOM	2987	CA	PHE	A	402	17.841	22.019	26.744	1.00	14.06	A	C
ATOM	2988	CB	PHE	A	402	17.401	22.853	25.517	1.00	14.70	A	C
ATOM	2989	CG	PHE	A	402	16.602	22.079	24.464	1.00	12.42	A	C
ATOM	2990	CD1	PHE	A	402	15.936	22.764	23.455	1.00	15.18	A	C
ATOM	2991	CE1	PHE	A	402	15.222	22.069	22.468	1.00	12.37	A	C
ATOM	2992	CZ	PHE	A	402	15.195	20.700	22.489	1.00	11.68	A	C
ATOM	2993	CE2	PHE	A	402	15.841	20.022	23.493	1.00	14.06	A	C
ATOM	2994	CD2	PHE	A	402	16.534	20.698	24.465	1.00	10.95	A	C
ATOM	2995	C	PHE	A	402	18.725	22.896	27.641	1.00	15.85	A	C
ATOM	2996	O	PHE	A	402	18.356	24.021	27.952	1.00	16.80	A	O
ATOM	2997	N	ILE	A	403	19.886	22.379	28.028	1.00	16.60	A	N
ATOM	2998	CA	ILE	A	403	20.787	23.062	28.963	1.00	17.41	A	C
ATOM	2999	CB	ILE	A	403	21.088	22.167	30.160	1.00	16.74	A	C
ATOM	3000	CG1	ILE	A	403	19.802	21.886	30.944	1.00	17.16	A	C
ATOM	3001	CD1	ILE	A	403	19.946	20.733	31.931	1.00	15.43	A	C
ATOM	3002	CG2	ILE	A	403	22.143	22.809	31.095	1.00	17.20	A	C
ATOM	3003	C	ILE	A	403	22.064	23.395	28.240	1.00	17.62	A	C
ATOM	3004	O	ILE	A	403	22.812	22.520	27.854	1.00	17.97	A	O
ATOM	3005	N	ASN	A	404	22.299	24.678	28.026	1.00	18.39	A	N
ATOM	3006	CA	ASN	A	404	23.429	25.112	27.231	1.00	19.61	A	C
ATOM	3007	CB	ASN	A	404	23.255	26.599	26.874	1.00	20.94	A	C
ATOM	3008	CG	ASN	A	404	24.297	27.071	25.913	1.00	26.59	A	C
ATOM	3009	OD1	ASN	A	404	24.339	26.618	24.752	1.00	32.24	A	O
ATOM	3010	ND2	ASN	A	404	25.177	27.980	26.381	1.00	32.91	A	N
ATOM	3011	C	ASN	A	404	24.773	24.892	27.940	1.00	18.94	A	C
ATOM	3012	O	ASN	A	404	25.769	24.575	27.296	1.00	18.69	A	O
ATOM	3013	N	ALA	A	405	24.779	25.020	29.262	1.00	18.60	A	N
ATOM	3014	CA	ALA	A	405	26.011	24.902	30.044	1.00	19.42	A	C
ATOM	3015	CB	ALA	A	405	26.450	26.317	30.582	1.00	19.40	A	C
ATOM	3016	C	ALA	A	405	25.787	23.934	31.217	1.00	19.12	A	C
ATOM	3017	O	ALA	A	405	25.582	24.364	32.360	1.00	18.74	A	O
ATOM	3018	N	PRO	A	406	25.782	22.632	30.936	1.00	19.16	A	N
ATOM	3019	CA	PRO	A	406	25.508	21.629	31.977	1.00	19.37	A	C
ATOM	3020	CB	PRO	A	406	25.266	20.351	31.156	1.00	19.25	A	C
ATOM	3021	CG	PRO	A	406	26.120	20.546	29.977	1.00	19.80	A	C
ATOM	3022	CD	PRO	A	406	26.033	22.010	29.631	1.00	18.90	A	C
ATOM	3023	C	PRO	A	406	26.689	21.437	32.923	1.00	19.45	A	C
ATOM	3024	O	PRO	A	406	27.815	21.833	32.607	1.00	19.95	A	O
ATOM	3025	N	GLN	A	407	26.437	20.819	34.072	1.00	19.97	A	N
ATOM	3026	CA	GLN	A	407	27.490	20.446	35.016	1.00	20.20	A	C
ATOM	3027	CB	GLN	A	407	26.908	20.387	36.413	1.00	21.02	A	C
ATOM	3028	CG	GLN	A	407	26.155	21.620	36.805	1.00	22.32	A	C
ATOM	3029	CD	GLN	A	407	25.122	21.323	37.849	1.00	23.76	A	C
ATOM	3030	OE1	GLN	A	407	25.320	20.443	38.713	1.00	21.20	A	O
ATOM	3031	NE2	GLN	A	407	24.016	22.040	37.789	1.00	22.99	A	N
ATOM	3032	C	GLN	A	407	28.062	19.075	34.675	1.00	20.27	A	C
ATOM	3033	O	GLN	A	407	27.392	18.232	34.057	1.00	19.75	A	O
ATOM	3034	N	SER	A	408	29.294	18.830	35.099	1.00	20.30	A	N
ATOM	3035	CA	SER	A	408	29.869	17.491	35.033	1.00	20.08	A	C
ATOM	3036	CB	SER	A	408	31.393	17.538	35.212	1.00	20.55	A	C
ATOM	3037	OG	SER	A	408	32.042	18.067	34.072	1.00	19.34	A	O
ATOM	3038	C	SER	A	408	29.269	16.615	36.120	1.00	19.97	A	C
ATOM	3039	O	SER	A	408	29.130	17.043	37.268	1.00	20.96	A	O
ATOM	3040	N	GLY	A	409	28.980	15.362	35.775	1.00	19.80	A	N
ATOM	3041	CA	GLY	A	409	28.447	14.392	36.715	1.00	18.94	A	C
ATOM	3042	C	GLY	A	409	27.216	13.697	36.160	1.00	19.28	A	C

ATOM	3043	O	GLY	A	409	27.026	13.646	34.940	1.00	18.32	A	O
ATOM	3044	N	THR	A	410	26.350	13.224	37.058	1.00	18.72	A	N
ATOM	3045	CA	THR	A	410	25.226	12.396	36.678	1.00	18.26	A	C
ATOM	3046	CB	THR	A	410	25.105	11.220	37.631	1.00	17.98	A	C
ATOM	3047	OG1	THR	A	410	26.334	10.466	37.637	1.00	16.34	A	O
ATOM	3048	CG2	THR	A	410	24.038	10.227	37.136	1.00	18.99	A	C
ATOM	3049	C	THR	A	410	23.923	13.183	36.687	1.00	18.19	A	C
ATOM	3050	O	THR	A	410	23.510	13.735	37.718	1.00	18.85	A	O
ATOM	3051	N	TYR	A	411	23.274	13.241	35.524	1.00	17.34	A	N
ATOM	3052	CA	TYR	A	411	21.942	13.783	35.430	1.00	16.46	A	C
ATOM	3053	CB	TYR	A	411	21.731	14.459	34.067	1.00	16.84	A	C
ATOM	3054	CG	TYR	A	411	22.286	15.869	34.025	1.00	16.33	A	C
ATOM	3055	CD1	TYR	A	411	21.458	16.953	34.156	1.00	16.27	A	C
ATOM	3056	CE1	TYR	A	411	21.956	18.231	34.131	1.00	16.41	A	C
ATOM	3057	CZ	TYR	A	411	23.319	18.438	33.994	1.00	17.03	A	C
ATOM	3058	OH	TYR	A	411	23.789	19.744	34.031	1.00	17.03	A	O
ATOM	3059	CE2	TYR	A	411	24.172	17.380	33.880	1.00	16.15	A	C
ATOM	3060	CD2	TYR	A	411	23.660	16.099	33.889	1.00	17.36	A	C
ATOM	3061	C	TYR	A	411	20.956	12.627	35.606	1.00	16.14	A	C
ATOM	3062	O	TYR	A	411	21.157	11.557	35.041	1.00	15.95	A	O
ATOM	3063	N	THR	A	412	19.920	12.841	36.399	1.00	15.50	A	N
ATOM	3064	CA	THR	A	412	18.760	11.959	36.418	1.00	16.39	A	C
ATOM	3065	CB	THR	A	412	18.107	12.037	37.808	1.00	16.73	A	C
ATOM	3066	OG1	THR	A	412	19.041	11.544	38.783	1.00	16.43	A	O
ATOM	3067	CG2	THR	A	412	16.877	11.115	37.946	1.00	18.16	A	C
ATOM	3068	C	THR	A	412	17.764	12.397	35.344	1.00	16.26	A	C
ATOM	3069	O	THR	A	412	17.404	13.568	35.286	1.00	15.84	A	O
ATOM	3070	N	VAL	A	413	17.313	11.444	34.516	1.00	16.67	A	N
ATOM	3071	CA	VAL	A	413	16.342	11.672	33.452	1.00	15.75	A	C
ATOM	3072	CB	VAL	A	413	16.924	11.246	32.066	1.00	16.41	A	C
ATOM	3073	CG1	VAL	A	413	15.914	11.476	30.914	1.00	15.53	A	C
ATOM	3074	CG2	VAL	A	413	18.240	11.946	31.773	1.00	15.42	A	C
ATOM	3075	C	VAL	A	413	15.134	10.811	33.791	1.00	16.95	A	C
ATOM	3076	O	VAL	A	413	15.232	9.574	33.667	1.00	18.21	A	O
ATOM	3077	N	GLU	A	414	14.040	11.439	34.256	1.00	16.21	A	N
ATOM	3078	CA	GLU	A	414	12.803	10.774	34.736	1.00	17.01	A	C
ATOM	3079	CB	GLU	A	414	12.467	11.202	36.134	1.00	16.06	A	C
ATOM	3080	CG	GLU	A	414	11.518	10.244	36.767	1.00	18.61	A	C
ATOM	3081	CD	GLU	A	414	11.626	10.318	38.265	1.00	17.99	A	C
ATOM	3082	OE1	GLU	A	414	11.212	11.334	38.830	1.00	20.38	A	O
ATOM	3083	OE2	GLU	A	414	12.198	9.404	38.810	1.00	18.55	A	O
ATOM	3084	C	GLU	A	414	11.715	11.142	33.729	1.00	16.05	A	C
ATOM	3085	O	GLU	A	414	11.428	12.301	33.528	1.00	15.27	A	O
ATOM	3086	N	VAL	A	415	11.037	10.172	33.145	1.00	16.93	A	N
ATOM	3087	CA	VAL	A	415	9.622	10.184	32.847	1.00	16.73	A	C
ATOM	3088	CB	VAL	A	415	9.472	9.367	31.526	1.00	17.17	A	C
ATOM	3089	CG1	VAL	A	415	8.168	9.660	30.813	1.00	16.00	A	C
ATOM	3090	CG2	VAL	A	415	10.652	9.660	30.622	1.00	16.72	A	C
ATOM	3091	C	VAL	A	415	8.540	9.769	33.787	1.00	16.71	A	C
ATOM	3092	O	VAL	A	415	8.463	8.634	34.185	1.00	16.19	A	O
ATOM	3093	N	GLN	A	416	7.684	10.736	34.077	1.00	16.05	A	N
ATOM	3094	CA	GLN	A	416	6.553	10.579	34.989	1.00	16.43	A	C
ATOM	3095	CB	GLN	A	416	6.519	11.747	35.981	1.00	16.01	A	C
ATOM	3096	CG	GLN	A	416	7.786	11.832	36.802	1.00	16.27	A	C
ATOM	3097	CD	GLN	A	416	7.821	12.929	37.827	1.00	17.22	A	C
ATOM	3098	OE1	GLN	A	416	6.912	13.762	37.905	1.00	16.47	A	O
ATOM	3099	NE2	GLN	A	416	8.933	12.972	38.601	1.00	16.72	A	N
ATOM	3100	C	GLN	A	416	5.232	10.504	34.235	1.00	17.01	A	C

ATOM	3101	O	GLN	A	416	4.899	11.388	33.440	1.00	16.94	A	O
ATOM	3102	N	ALA	A	417	4.461	9.462	34.522	1.00	17.66	A	N
ATOM	3103	CA	ALA	A	417	3.122	9.307	33.953	1.00	18.17	A	C
ATOM	3104	CB	ALA	A	417	2.770	7.857	33.891	1.00	18.16	A	C
ATOM	3105	C	ALA	A	417	2.092	10.083	34.790	1.00	19.19	A	C
ATOM	3106	O	ALA	A	417	1.542	9.565	35.775	1.00	18.61	A	O
ATOM	3107	N	TYR	A	418	1.859	11.338	34.437	1.00	19.27	A	N
ATOM	3108	CA	TYR	A	418	0.944	12.153	35.234	1.00	20.10	A	C
ATOM	3109	CB	TYR	A	418	0.985	13.618	34.803	1.00	20.65	A	C
ATOM	3110	CG	TYR	A	418	0.021	14.496	35.570	1.00	23.36	A	C
ATOM	3111	CD1	TYR	A	418	0.255	14.818	36.908	1.00	26.20	A	C
ATOM	3112	CE1	TYR	A	418	-0.645	15.610	37.625	1.00	29.96	A	C
ATOM	3113	CZ	TYR	A	418	-1.772	16.099	36.990	1.00	31.45	A	C
ATOM	3114	OH	TYR	A	418	-2.659	16.888	37.685	1.00	34.45	A	O
ATOM	3115	CE2	TYR	A	418	-2.018	15.804	35.652	1.00	29.32	A	C
ATOM	3116	CD2	TYR	A	418	-1.123	15.002	34.957	1.00	26.35	A	C
ATOM	3117	C	TYR	A	418	-0.477	11.623	35.158	1.00	19.95	A	C
ATOM	3118	O	TYR	A	418	-1.142	11.445	36.190	1.00	19.83	A	O
ATOM	3119	N	ASN	A	419	-0.928	11.332	33.945	1.00	19.39	A	N
ATOM	3120	CA	ASN	A	419	-2.284	10.855	33.708	1.00	19.40	A	C
ATOM	3121	CB	ASN	A	419	-3.243	12.051	33.629	1.00	20.03	A	C
ATOM	3122	CG	ASN	A	419	-4.705	11.625	33.611	1.00	21.53	A	C
ATOM	3123	OD1	ASN	A	419	-5.094	10.758	34.354	1.00	23.42	A	O
ATOM	3124	ND2	ASN	A	419	-5.493	12.212	32.727	1.00	22.67	A	N
ATOM	3125	C	ASN	A	419	-2.374	10.079	32.402	1.00	19.75	A	C
ATOM	3126	O	ASN	A	419	-2.186	10.646	31.317	1.00	19.24	A	O
ATOM	3127	N	VAL	A	420	-2.703	8.795	32.486	1.00	19.24	A	N
ATOM	3128	CA	VAL	A	420	-2.744	7.948	31.295	1.00	18.57	A	C
ATOM	3129	CB	VAL	A	420	-1.533	6.986	31.288	1.00	18.55	A	C
ATOM	3130	CG1	VAL	A	420	-1.504	6.086	30.040	1.00	17.15	A	C
ATOM	3131	CG2	VAL	A	420	-0.196	7.799	31.402	1.00	20.43	A	C
ATOM	3132	C	VAL	A	420	-4.067	7.165	31.234	1.00	18.55	A	C
ATOM	3133	O	VAL	A	420	-4.109	5.996	31.606	1.00	18.55	A	O
ATOM	3134	N	PRO	A	421	-5.132	7.816	30.776	1.00	18.79	A	N
ATOM	3135	CA	PRO	A	421	-6.444	7.169	30.635	1.00	19.54	A	C
ATOM	3136	CB	PRO	A	421	-7.397	8.324	30.288	1.00	19.65	A	C
ATOM	3137	CG	PRO	A	421	-6.540	9.394	29.746	1.00	19.70	A	C
ATOM	3138	CD	PRO	A	421	-5.175	9.239	30.396	1.00	18.68	A	C
ATOM	3139	C	PRO	A	421	-6.507	6.141	29.530	1.00	19.68	A	C
ATOM	3140	O	PRO	A	421	-7.411	5.318	29.565	1.00	20.15	A	O
ATOM	3141	N	VAL	A	422	-5.592	6.178	28.566	1.00	19.04	A	N
ATOM	3142	CA	VAL	A	422	-5.594	5.180	27.505	1.00	18.85	A	C
ATOM	3143	CB	VAL	A	422	-5.990	5.781	26.146	1.00	18.35	A	C
ATOM	3144	CG1	VAL	A	422	-6.200	4.653	25.091	1.00	18.91	A	C
ATOM	3145	CG2	VAL	A	422	-7.264	6.616	26.285	1.00	18.28	A	C
ATOM	3146	C	VAL	A	422	-4.226	4.509	27.448	1.00	19.38	A	C
ATOM	3147	O	VAL	A	422	-3.435	4.713	26.505	1.00	18.38	A	O
ATOM	3148	N	GLY	A	423	-3.957	3.707	28.480	1.00	19.46	A	N
ATOM	3149	CA	GLY	A	423	-2.642	3.150	28.702	1.00	19.62	A	C
ATOM	3150	C	GLY	A	423	-2.510	1.665	28.496	1.00	19.72	A	C
ATOM	3151	O	GLY	A	423	-3.464	0.954	28.162	1.00	21.71	A	O
ATOM	3152	N	PRO	A	424	-1.307	1.174	28.695	1.00	19.10	A	N
ATOM	3153	CA	PRO	A	424	-0.142	1.999	29.040	1.00	17.55	A	C
ATOM	3154	CB	PRO	A	424	0.876	0.969	29.467	1.00	18.01	A	C
ATOM	3155	CG	PRO	A	424	0.510	-0.258	28.696	1.00	19.87	A	C
ATOM	3156	CD	PRO	A	424	-0.988	-0.267	28.649	1.00	19.26	A	C
ATOM	3157	C	PRO	A	424	0.396	2.842	27.899	1.00	16.87	A	C
ATOM	3158	O	PRO	A	424	0.038	2.660	26.733	1.00	17.20	A	O



ATOM	3159	N	GLN	A	425	1.248	3.798	28.239	1.00	15.38	A	N
ATOM	3160	CA	GLN	A	425	1.848	4.678	27.240	1.00	14.36	A	C
ATOM	3161	CB	GLN	A	425	1.507	6.140	27.559	1.00	14.88	A	C
ATOM	3162	CG	GLN	A	425	2.070	7.202	26.576	1.00	14.70	A	C
ATOM	3163	CD	GLN	A	425	1.512	7.043	25.180	1.00	16.71	A	C
ATOM	3164	OE1	GLN	A	425	0.321	7.321	24.956	1.00	15.27	A	O
ATOM	3165	NE2	GLN	A	425	2.349	6.580	24.235	1.00	11.93	A	N
ATOM	3166	C	GLN	A	425	3.341	4.470	27.252	1.00	13.10	A	C
ATOM	3167	O	GLN	A	425	3.987	4.662	28.283	1.00	12.18	A	O
ATOM	3168	N	THR	A	426	3.887	4.036	26.112	1.00	12.88	A	N
ATOM	3169	CA	THR	A	426	5.320	4.008	25.913	1.00	12.90	A	C
ATOM	3170	CB	THR	A	426	5.737	2.949	24.890	1.00	12.37	A	C
ATOM	3171	OG1	THR	A	426	5.134	3.254	23.626	1.00	12.70	A	O
ATOM	3172	CG2	THR	A	426	5.232	1.573	25.283	1.00	13.56	A	C
ATOM	3173	C	THR	A	426	5.796	5.370	25.413	1.00	13.16	A	C
ATOM	3174	O	THR	A	426	4.986	6.223	25.037	1.00	14.38	A	O
ATOM	3175	N	PHE	A	427	7.115	5.551	25.401	1.00	12.86	A	N
ATOM	3176	CA	PHE	A	427	7.741	6.823	25.036	1.00	12.44	A	C
ATOM	3177	CB	PHE	A	427	7.802	7.778	26.240	1.00	12.42	A	C
ATOM	3178	CG	PHE	A	427	8.612	7.235	27.366	1.00	12.82	A	C
ATOM	3179	CD1	PHE	A	427	9.988	7.361	27.365	1.00	15.21	A	C
ATOM	3180	CE1	PHE	A	427	10.768	6.801	28.381	1.00	15.74	A	C
ATOM	3181	CZ	PHE	A	427	10.161	6.102	29.408	1.00	14.88	A	C
ATOM	3182	CE2	PHE	A	427	8.766	5.987	29.427	1.00	16.39	A	C
ATOM	3183	CD2	PHE	A	427	8.000	6.538	28.407	1.00	14.33	A	C
ATOM	3184	C	PHE	A	427	9.149	6.532	24.549	1.00	12.14	A	C
ATOM	3185	O	PHE	A	427	9.694	5.444	24.807	1.00	11.55	A	O
ATOM	3186	N	SER	A	428	9.721	7.523	23.867	1.00	11.59	A	N
ATOM	3187	CA	SER	A	428	11.116	7.528	23.480	1.00	11.99	A	C
ATOM	3188	CB	SER	A	428	11.292	7.463	21.965	1.00	12.17	A	C
ATOM	3189	OG	SER	A	428	10.837	6.219	21.442	1.00	12.32	A	O
ATOM	3190	C	SER	A	428	11.804	8.776	24.031	1.00	12.57	A	C
ATOM	3191	O	SER	A	428	11.174	9.829	24.263	1.00	11.91	A	O
ATOM	3192	N	LEU	A	429	13.103	8.620	24.278	1.00	12.35	A	N
ATOM	3193	CA	LEU	A	429	13.950	9.712	24.714	1.00	12.57	A	C
ATOM	3194	CB	LEU	A	429	14.508	9.476	26.135	1.00	12.84	A	C
ATOM	3195	CG	LEU	A	429	13.542	9.648	27.296	1.00	13.77	A	C
ATOM	3196	CD1	LEU	A	429	14.046	8.907	28.520	1.00	15.69	A	C
ATOM	3197	CD2	LEU	A	429	13.348	11.110	27.609	1.00	15.64	A	C
ATOM	3198	C	LEU	A	429	15.098	9.756	23.768	1.00	11.82	A	C
ATOM	3199	O	LEU	A	429	15.593	8.707	23.372	1.00	11.44	A	O
ATOM	3200	N	ALA	A	430	15.532	10.957	23.405	1.00	11.55	A	N
ATOM	3201	CA	ALA	A	430	16.805	11.139	22.699	1.00	11.87	A	C
ATOM	3202	CB	ALA	A	430	16.581	11.528	21.235	1.00	12.63	A	C
ATOM	3203	C	ALA	A	430	17.613	12.215	23.404	1.00	12.76	A	C
ATOM	3204	O	ALA	A	430	17.072	13.256	23.776	1.00	12.14	A	O
ATOM	3205	N	ILE	A	431	18.907	11.943	23.584	1.00	12.52	A	N
ATOM	3206	CA	ILE	A	431	19.813	12.835	24.287	1.00	13.32	A	C
ATOM	3207	CB	ILE	A	431	20.325	12.179	25.593	1.00	13.00	A	C
ATOM	3208	CG1	ILE	A	431	19.175	11.882	26.542	1.00	14.30	A	C
ATOM	3209	CD1	ILE	A	431	19.575	11.061	27.776	1.00	16.21	A	C
ATOM	3210	CG2	ILE	A	431	21.292	13.123	26.288	1.00	14.86	A	C
ATOM	3211	C	ILE	A	431	21.005	13.176	23.392	1.00	12.92	A	C
ATOM	3212	O	ILE	A	431	21.728	12.288	22.937	1.00	11.26	A	O
ATOM	3213	N	VAL	A	432	21.192	14.464	23.134	1.00	13.80	A	N
ATOM	3214	CA	VAL	A	432	22.387	14.966	22.483	1.00	15.20	A	C
ATOM	3215	CB	VAL	A	432	22.028	15.996	21.387	1.00	15.89	A	C
ATOM	3216	CG1	VAL	A	432	23.293	16.591	20.809	1.00	15.25	A	C



ATOM	3217	CG2	VAL	A	432	21.167	15.361	20.293	1.00	15.39	A	C
ATOM	3218	C	VAL	A	432	23.346	15.634	23.498	1.00	16.38	A	C
ATOM	3219	O	VAL	A	432	22.923	16.472	24.298	1.00	16.49	A	O
ATOM	3220	N	HIS	A	433	24.633	15.257	23.458	1.00	17.45	A	N
ATOM	3221	CA	HIS	A	433	25.669	15.872	24.306	1.00	18.55	A	C
ATOM	3222	CB	HIS	A	433	25.637	15.240	25.711	1.00	19.21	A	C
ATOM	3223	CG	HIS	A	433	26.553	15.885	26.707	1.00	19.32	A	C
ATOM	3224	ND1	HIS	A	433	26.497	17.233	27.015	1.00	18.22	A	N
ATOM	3225	CE1	HIS	A	433	27.378	17.497	27.969	1.00	18.90	A	C
ATOM	3226	NE2	HIS	A	433	27.999	16.380	28.289	1.00	16.51	A	N
ATOM	3227	CD2	HIS	A	433	27.502	15.353	27.513	1.00	17.65	A	C
ATOM	3228	C	HIS	A	433	27.031	15.627	23.684	1.00	19.74	A	C
ATOM	3229	O	HIS	A	433	27.664	16.546	23.133	1.00	21.68	A	O
ATOM	3230	OXT	HIS	A	433	27.463	14.480	23.735	1.00	19.29	A	O
TER	3230		HIS	A	433							
HETATM	3231	CA	CA	A	601	15.429	35.876	3.369	1.00	16.92	A	CA
HETATM	3232	CA	CA	A	602	3.346	16.597	30.346	1.00	13.45	A	CA
HETATM	3233	CA	CA	A	603	9.615	28.353	34.891	1.00	17.30	A	CA
ATOM	3234	N	ASP	B	16	3.955	53.303	-10.201	1.00	49.01	B	N
ATOM	3235	CA	ASP	B	16	4.171	51.870	-9.771	1.00	49.32	B	C
ATOM	3236	CB	ASP	B	16	5.553	51.425	-10.270	1.00	49.78	B	C
ATOM	3237	CG	ASP	B	16	6.176	52.438	-11.248	1.00	52.12	B	C
ATOM	3238	OD1	ASP	B	16	5.667	52.549	-12.399	1.00	54.86	B	O
ATOM	3239	OD2	ASP	B	16	7.151	53.181	-10.957	1.00	52.51	B	O
ATOM	3240	C	ASP	B	16	4.009	51.690	-8.232	1.00	48.45	B	C
ATOM	3241	O	ASP	B	16	4.793	50.996	-7.567	1.00	47.87	B	O
ATOM	3242	N	ARG	B	17	2.959	52.301	-7.687	1.00	47.87	B	N
ATOM	3243	CA	ARG	B	17	2.863	52.592	-6.247	1.00	47.30	B	C
ATOM	3244	CB	ARG	B	17	2.430	54.064	-6.059	1.00	46.77	B	C
ATOM	3245	CG	ARG	B	17	3.107	55.055	-7.028	1.00	44.50	B	C
ATOM	3246	CD	ARG	B	17	2.860	56.528	-6.691	1.00	39.98	B	C
ATOM	3247	NE	ARG	B	17	3.266	56.891	-5.335	1.00	33.05	B	N
ATOM	3248	CZ	ARG	B	17	4.483	57.334	-5.001	1.00	29.36	B	C
ATOM	3249	NH1	ARG	B	17	5.440	57.459	-5.915	1.00	28.07	B	N
ATOM	3250	NH2	ARG	B	17	4.752	57.650	-3.740	1.00	24.57	B	N
ATOM	3251	C	ARG	B	17	1.917	51.699	-5.415	1.00	48.01	B	C
ATOM	3252	O	ARG	B	17	1.463	52.120	-4.342	1.00	47.42	B	O
ATOM	3253	N	HIS	B	18	1.616	50.486	-5.885	1.00	48.51	B	N
ATOM	3254	CA	HIS	B	18	0.770	49.573	-5.108	1.00	48.98	B	C
ATOM	3255	CB	HIS	B	18	0.515	48.266	-5.875	1.00	49.29	B	C
ATOM	3256	CG	HIS	B	18	-0.510	48.388	-6.961	1.00	50.05	B	C
ATOM	3257	ND1	HIS	B	18	-0.195	48.803	-8.238	1.00	51.24	B	N
ATOM	3258	CE1	HIS	B	18	-1.291	48.814	-8.979	1.00	51.27	B	C
ATOM	3259	NE2	HIS	B	18	-2.305	48.419	-8.228	1.00	50.69	B	N
ATOM	3260	CD2	HIS	B	18	-1.844	48.147	-6.962	1.00	50.64	B	C
ATOM	3261	C	HIS	B	18	1.429	49.229	-3.770	1.00	49.16	B	C
ATOM	3262	O	HIS	B	18	2.598	48.822	-3.738	1.00	49.03	B	O
ATOM	3263	N	ASN	B	19	0.690	49.386	-2.667	1.00	49.15	B	N
ATOM	3264	CA	ASN	B	19	1.167	48.868	-1.384	1.00	49.11	B	C
ATOM	3265	CB	ASN	B	19	0.276	49.313	-0.205	1.00	49.60	B	C
ATOM	3266	CG	ASN	B	19	0.951	49.099	1.176	1.00	51.24	B	C
ATOM	3267	OD1	ASN	B	19	0.415	48.415	2.058	1.00	53.59	B	O
ATOM	3268	ND2	ASN	B	19	2.123	49.705	1.363	1.00	54.56	B	N
ATOM	3269	C	ASN	B	19	1.241	47.332	-1.459	1.00	48.22	B	C
ATOM	3270	O	ASN	B	19	0.443	46.685	-2.138	1.00	47.43	B	O
ATOM	3271	N	LEU	B	20	2.221	46.772	-0.762	1.00	47.20	B	N
ATOM	3272	CA	LEU	B	20	2.393	45.333	-0.689	1.00	46.38	B	C
ATOM	3273	CB	LEU	B	20	3.743	45.000	-0.055	1.00	46.97	B	C

ATOM	3274	CG	LEU	B	20	4.896	45.800	-0.684	1.00	48.40	B	C
ATOM	3275	CD1	LEU	B	20	6.201	45.666	0.117	1.00	49.54	B	C
ATOM	3276	CD2	LEU	B	20	5.076	45.391	-2.158	1.00	48.69	B	C
ATOM	3277	C	LEU	B	20	1.235	44.792	0.141	1.00	44.75	B	C
ATOM	3278	O	LEU	B	20	1.113	45.092	1.342	1.00	45.26	B	O
ATOM	3279	N	LYS	B	21	0.338	44.073	-0.523	1.00	41.97	B	N
ATOM	3280	CA	LYS	B	21	-0.740	43.395	0.170	1.00	39.98	B	C
ATOM	3281	CB	LYS	B	21	-2.088	44.025	-0.183	1.00	40.54	B	C
ATOM	3282	CG	LYS	B	21	-3.225	43.550	0.700	1.00	41.63	B	C
ATOM	3283	CD	LYS	B	21	-4.257	44.620	0.878	1.00	43.44	B	C
ATOM	3284	CE	LYS	B	21	-5.391	44.131	1.718	1.00	44.82	B	C
ATOM	3285	NZ	LYS	B	21	-4.992	44.004	3.147	1.00	47.17	B	N
ATOM	3286	C	LYS	B	21	-0.710	41.917	-0.214	1.00	37.09	B	C
ATOM	3287	O	LYS	B	21	-0.679	41.588	-1.395	1.00	35.80	B	O
ATOM	3288	N	THR	B	22	-0.685	41.045	0.796	1.00	33.91	B	N
ATOM	3289	CA	THR	B	22	-0.642	39.592	0.593	1.00	31.44	B	C
ATOM	3290	CB	THR	B	22	0.734	39.046	1.030	1.00	31.70	B	C
ATOM	3291	OG1	THR	B	22	1.002	39.436	2.387	1.00	31.47	B	O
ATOM	3292	CG2	THR	B	22	1.857	39.681	0.211	1.00	31.30	B	C
ATOM	3293	C	THR	B	22	-1.739	38.843	1.342	1.00	29.57	B	C
ATOM	3294	O	THR	B	22	-1.830	37.617	1.246	1.00	28.17	B	O
ATOM	3295	N	GLU	B	23	-2.542	39.576	2.107	1.00	27.46	B	N
ATOM	3296	CA	GLU	B	23	-3.672	39.011	2.828	1.00	27.22	B	C
ATOM	3297	CB	BGLU	B	23	-3.280	38.728	4.282	0.50	27.51	B	C
ATOM	3298	CB	AGLU	B	23	-3.287	38.646	4.277	0.50	27.17	B	C
ATOM	3299	CG	BGLU	B	23	-2.826	37.304	4.512	0.50	29.10	B	C
ATOM	3300	CG	AGLU	B	23	-3.050	39.822	5.223	0.50	27.55	B	C
ATOM	3301	CD	BGLU	B	23	-2.236	37.062	5.891	0.50	30.84	B	C
ATOM	3302	CD	AGLU	B	23	-3.020	39.396	6.689	0.50	28.07	B	C
ATOM	3303	OE1	BGLU	B	23	-1.959	38.040	6.614	0.50	32.02	B	O
ATOM	3304	OE1	AGLU	B	23	-2.853	38.186	6.954	0.50	28.41	B	O
ATOM	3305	OE2	BGLU	B	23	-2.054	35.879	6.241	0.50	31.16	B	O
ATOM	3306	OE2	AGLU	B	23	-3.182	40.264	7.579	0.50	28.60	B	O
ATOM	3307	C	GLU	B	23	-4.842	39.988	2.799	1.00	25.94	B	C
ATOM	3308	O	GLU	B	23	-4.631	41.199	2.805	1.00	25.17	B	O
ATOM	3309	N	TRP	B	24	-6.065	39.462	2.765	1.00	24.57	B	N
ATOM	3310	CA	TRP	B	24	-7.264	40.300	2.708	1.00	23.89	B	C
ATOM	3311	CB	TRP	B	24	-7.910	40.174	1.304	1.00	23.59	B	C
ATOM	3312	CG	TRP	B	24	-7.105	40.786	0.245	1.00	21.71	B	C
ATOM	3313	CD1	TRP	B	24	-7.232	42.050	-0.239	1.00	21.02	B	C
ATOM	3314	NE1	TRP	B	24	-6.293	42.276	-1.211	1.00	18.62	B	N
ATOM	3315	CE2	TRP	B	24	-5.544	41.148	-1.396	1.00	19.02	B	C
ATOM	3316	CD2	TRP	B	24	-6.006	40.190	-0.480	1.00	20.72	B	C
ATOM	3317	CE3	TRP	B	24	-5.387	38.941	-0.454	1.00	19.49	B	C
ATOM	3318	CZ3	TRP	B	24	-4.326	38.694	-1.313	1.00	20.25	B	C
ATOM	3319	CH2	TRP	B	24	-3.883	39.662	-2.207	1.00	21.63	B	C
ATOM	3320	CZ2	TRP	B	24	-4.477	40.911	-2.257	1.00	22.09	B	C
ATOM	3321	C	TRP	B	24	-8.294	39.948	3.789	1.00	23.91	B	C
ATOM	3322	O	TRP	B	24	-9.369	39.456	3.467	1.00	22.74	B	O
ATOM	3323	N	PRO	B	25	-7.986	40.196	5.070	1.00	24.64	B	N
ATOM	3324	CA	PRO	B	25	-8.918	39.850	6.161	1.00	25.12	B	C
ATOM	3325	CB	PRO	B	25	-8.176	40.312	7.448	1.00	25.87	B	C
ATOM	3326	CG	PRO	B	25	-7.011	41.163	7.002	1.00	26.08	B	C
ATOM	3327	CD	PRO	B	25	-6.737	40.807	5.562	1.00	25.49	B	C
ATOM	3328	C	PRO	B	25	-10.307	40.520	6.029	1.00	25.18	B	C
ATOM	3329	O	PRO	B	25	-11.310	39.978	6.469	1.00	24.94	B	O
ATOM	3330	N	GLU	B	26	-10.350	41.668	5.364	1.00	25.43	B	N
ATOM	3331	CA	GLU	B	26	-11.581	42.416	5.141	1.00	25.93	B	C

ATOM	3332	CB	GLU	B	26	-11.243	43.829	4.627	1.00	26.70	B	C
ATOM	3333	CG	GLU	B	26	-10.690	43.922	3.189	1.00	28.62	B	C
ATOM	3334	CD	GLU	B	26	-9.169	43.775	3.077	1.00	29.61	B	C
ATOM	3335	OE1	GLU	B	26	-8.535	43.174	3.985	1.00	28.68	B	O
ATOM	3336	OE2	GLU	B	26	-8.608	44.252	2.057	1.00	31.71	B	O
ATOM	3337	C	GLU	B	26	-12.571	41.705	4.193	1.00	25.60	B	C
ATOM	3338	O	GLU	B	26	-13.746	42.060	4.139	1.00	24.75	B	O
ATOM	3339	N	LEU	B	27	-12.119	40.672	3.483	1.00	24.52	B	N
ATOM	3340	CA	LEU	B	27	-12.957	40.024	2.483	1.00	23.54	B	C
ATOM	3341	CB	LEU	B	27	-12.104	39.593	1.287	1.00	23.84	B	C
ATOM	3342	CG	LEU	B	27	-11.506	40.722	0.430	1.00	23.08	B	C
ATOM	3343	CD1	LEU	B	27	-10.702	40.165	-0.732	1.00	22.31	B	C
ATOM	3344	CD2	LEU	B	27	-12.603	41.624	-0.097	1.00	23.37	B	C
ATOM	3345	C	LEU	B	27	-13.716	38.829	3.042	1.00	23.75	B	C
ATOM	3346	O	LEU	B	27	-14.504	38.205	2.334	1.00	23.33	B	O
ATOM	3347	N	VAL	B	28	-13.490	38.504	4.312	1.00	23.89	B	N
ATOM	3348	CA	VAL	B	28	-14.143	37.357	4.918	1.00	24.64	B	C
ATOM	3349	CB	VAL	B	28	-13.571	37.050	6.359	1.00	24.78	B	C
ATOM	3350	CG1	VAL	B	28	-14.359	35.963	7.027	1.00	25.39	B	C
ATOM	3351	CG2	VAL	B	28	-12.099	36.634	6.272	1.00	25.78	B	C
ATOM	3352	C	VAL	B	28	-15.612	37.694	4.992	1.00	24.75	B	C
ATOM	3353	O	VAL	B	28	-15.952	38.791	5.424	1.00	25.68	B	O
ATOM	3354	N	GLY	B	29	-16.468	36.797	4.516	1.00	24.86	B	N
ATOM	3355	CA	GLY	B	29	-17.916	37.000	4.539	1.00	24.80	B	C
ATOM	3356	C	GLY	B	29	-18.493	37.638	3.274	1.00	25.07	B	C
ATOM	3357	O	GLY	B	29	-19.692	37.598	3.061	1.00	25.27	B	O
ATOM	3358	N	LYS	B	30	-17.630	38.203	2.429	1.00	25.21	B	N
ATOM	3359	CA	LYS	B	30	-18.025	38.782	1.146	1.00	24.62	B	C
ATOM	3360	CB	LYS	B	30	-16.952	39.780	0.679	1.00	25.65	B	C
ATOM	3361	CG	LYS	B	30	-16.716	40.964	1.606	1.00	28.42	B	C
ATOM	3362	CD	LYS	B	30	-16.577	42.245	0.785	1.00	34.26	B	C
ATOM	3363	CE	LYS	B	30	-16.462	43.527	1.631	1.00	35.92	B	C
ATOM	3364	NZ	LYS	B	30	-15.996	43.273	3.011	1.00	37.72	B	N
ATOM	3365	C	LYS	B	30	-18.188	37.728	0.065	1.00	23.30	B	C
ATOM	3366	O	LYS	B	30	-17.670	36.623	0.166	1.00	22.29	B	O
ATOM	3367	N	SER	B	31	-18.884	38.089	-1.001	1.00	21.94	B	N
ATOM	3368	CA	SER	B	31	-19.036	37.204	-2.145	1.00	20.89	B	C
ATOM	3369	CB	SER	B	31	-20.046	37.776	-3.143	1.00	21.21	B	C
ATOM	3370	OG	SER	B	31	-19.519	38.912	-3.815	1.00	20.40	B	O
ATOM	3371	C	SER	B	31	-17.726	37.017	-2.865	1.00	19.88	B	C
ATOM	3372	O	SER	B	31	-16.828	37.843	-2.800	1.00	18.67	B	O
ATOM	3373	N	VAL	B	32	-17.649	35.920	-3.588	1.00	20.34	B	N
ATOM	3374	CA	VAL	B	32	-16.487	35.617	-4.393	1.00	20.89	B	C
ATOM	3375	CB	BVAL	B	32	-16.717	34.256	-5.141	0.50	20.94	B	C
ATOM	3376	CB	AVAL	B	32	-16.555	34.234	-5.043	0.50	21.07	B	C
ATOM	3377	CG1	BVAL	B	32	-16.023	34.221	-6.524	0.50	20.85	B	C
ATOM	3378	CG1	AVAL	B	32	-17.648	34.180	-6.069	0.50	20.79	B	C
ATOM	3379	CG2	BVAL	B	32	-16.276	33.087	-4.281	0.50	20.73	B	C
ATOM	3380	CG2	AVAL	B	32	-15.193	33.903	-5.657	0.50	21.36	B	C
ATOM	3381	C	VAL	B	32	-16.238	36.732	-5.431	1.00	20.83	B	C
ATOM	3382	O	VAL	B	32	-15.100	37.105	-5.681	1.00	20.37	B	O
ATOM	3383	N	GLU	B	33	-17.316	37.263	-6.011	1.00	21.19	B	N
ATOM	3384	CA	GLU	B	33	-17.205	38.264	-7.072	1.00	21.20	B	C
ATOM	3385	CB	GLU	B	33	-18.553	38.478	-7.767	1.00	21.59	B	C
ATOM	3386	CG	GLU	B	33	-19.045	37.271	-8.543	1.00	24.67	B	C
ATOM	3387	CD	GLU	B	33	-19.799	36.219	-7.708	1.00	29.01	B	C
ATOM	3388	OE1	GLU	B	33	-20.001	35.123	-8.275	1.00	36.54	B	O
ATOM	3389	OE2	GLU	B	33	-20.187	36.437	-6.517	1.00	27.78	B	O

ATOM	3390	C	GLU	B	33	-16.688	39.571	-6.497	1.00	20.62	B	C
ATOM	3391	O	GLU	B	33	-15.885	40.255	-7.130	1.00	20.20	B	O
ATOM	3392	N	GLU	B	34	-17.124	39.910	-5.283	1.00	20.61	B	N
ATOM	3393	CA	GLU	B	34	-16.627	41.131	-4.634	1.00	20.97	B	C
ATOM	3394	CB	GLU	B	34	-17.456	41.533	-3.407	1.00	21.10	B	C
ATOM	3395	CG	GLU	B	34	-18.778	42.224	-3.722	1.00	25.82	B	C
ATOM	3396	CD	GLU	B	34	-18.615	43.546	-4.481	1.00	31.16	B	C
ATOM	3397	OE1	GLU	B	34	-17.968	44.484	-3.932	1.00	32.84	B	O
ATOM	3398	OE2	GLU	B	34	-19.135	43.645	-5.626	1.00	33.71	B	O
ATOM	3399	C	GLU	B	34	-15.156	40.951	-4.257	1.00	19.67	B	C
ATOM	3400	O	GLU	B	34	-14.340	41.858	-4.438	1.00	18.91	B	O
ATOM	3401	N	ALA	B	35	-14.809	39.775	-3.765	1.00	19.75	B	N
ATOM	3402	CA	ALA	B	35	-13.414	39.485	-3.401	1.00	19.10	B	C
ATOM	3403	CB	ALA	B	35	-13.311	38.127	-2.749	1.00	19.66	B	C
ATOM	3404	C	ALA	B	35	-12.457	39.581	-4.582	1.00	18.90	B	C
ATOM	3405	O	ALA	B	35	-11.387	40.183	-4.470	1.00	18.82	B	O
ATOM	3406	N	LYS	B	36	-12.839	38.993	-5.716	1.00	18.68	B	N
ATOM	3407	CA	LYS	B	36	-11.991	38.978	-6.894	1.00	18.17	B	C
ATOM	3408	CB	LYS	B	36	-12.659	38.220	-8.063	1.00	18.44	B	C
ATOM	3409	CG	LYS	B	36	-12.714	36.693	-7.928	1.00	19.56	B	C
ATOM	3410	CD	LYS	B	36	-13.304	36.026	-9.159	1.00	20.72	B	C
ATOM	3411	CE	LYS	B	36	-13.194	34.496	-9.136	1.00	22.32	B	C
ATOM	3412	NZ	LYS	B	36	-13.963	33.865	-10.274	1.00	20.54	B	N
ATOM	3413	C	LYS	B	36	-11.648	40.406	-7.316	1.00	17.67	B	C
ATOM	3414	O	LYS	B	36	-10.500	40.694	-7.681	1.00	17.81	B	O
ATOM	3415	N	LYS	B	37	-12.614	41.316	-7.254	1.00	17.52	B	N
ATOM	3416	CA	LYS	B	37	-12.345	42.667	-7.746	1.00	17.89	B	C
ATOM	3417	CB	LYS	B	37	-13.621	43.519	-7.870	1.00	17.35	B	C
ATOM	3418	CG	LYS	B	37	-14.544	43.165	-9.036	1.00	17.43	B	C
ATOM	3419	CD	LYS	B	37	-15.847	44.074	-9.064	1.00	15.06	B	C
ATOM	3420	CE	LYS	B	37	-16.801	43.812	-7.921	1.00	16.48	B	C
ATOM	3421	NZ	LYS	B	37	-18.031	44.685	-7.989	1.00	15.66	B	N
ATOM	3422	C	LYS	B	37	-11.333	43.372	-6.852	1.00	18.04	B	C
ATOM	3423	O	LYS	B	37	-10.499	44.126	-7.354	1.00	18.33	B	O
ATOM	3424	N	VAL	B	38	-11.436	43.174	-5.535	1.00	17.93	B	N
ATOM	3425	CA	VAL	B	38	-10.525	43.824	-4.595	1.00	18.53	B	C
ATOM	3426	CB	VAL	B	38	-11.024	43.636	-3.136	1.00	19.32	B	C
ATOM	3427	CG1	VAL	B	38	-9.975	44.055	-2.128	1.00	21.52	B	C
ATOM	3428	CG2	VAL	B	38	-12.310	44.445	-2.919	1.00	20.73	B	C
ATOM	3429	C	VAL	B	38	-9.122	43.270	-4.742	1.00	18.91	B	C
ATOM	3430	O	VAL	B	38	-8.135	44.013	-4.797	1.00	17.79	B	O
ATOM	3431	N	ILE	B	39	-9.033	41.947	-4.830	1.00	19.11	B	N
ATOM	3432	CA	ILE	B	39	-7.747	41.304	-5.009	1.00	19.64	B	C
ATOM	3433	CB	ILE	B	39	-7.919	39.764	-4.973	1.00	19.43	B	C
ATOM	3434	CG1	ILE	B	39	-8.288	39.324	-3.573	1.00	20.37	B	C
ATOM	3435	CD1	ILE	B	39	-8.994	37.995	-3.564	1.00	21.36	B	C
ATOM	3436	CG2	ILE	B	39	-6.657	39.024	-5.470	1.00	19.76	B	C
ATOM	3437	C	ILE	B	39	-7.077	41.759	-6.287	1.00	19.71	B	C
ATOM	3438	O	ILE	B	39	-5.877	42.087	-6.266	1.00	19.70	B	O
ATOM	3439	N	LEU	B	40	-7.816	41.785	-7.404	1.00	19.22	B	N
ATOM	3440	CA	LEU	B	40	-7.205	42.231	-8.664	1.00	19.62	B	C
ATOM	3441	CB	LEU	B	40	-8.100	41.927	-9.888	1.00	19.18	B	C
ATOM	3442	CG	LEU	B	40	-8.145	40.416	-10.190	1.00	20.23	B	C
ATOM	3443	CD1	LEU	B	40	-9.235	40.047	-11.123	1.00	19.43	B	C
ATOM	3444	CD2	LEU	B	40	-6.799	39.947	-10.725	1.00	21.26	B	C
ATOM	3445	C	LEU	B	40	-6.840	43.716	-8.608	1.00	19.20	B	C
ATOM	3446	O	LEU	B	40	-5.939	44.144	-9.300	1.00	19.48	B	O
ATOM	3447	N	GLN	B	41	-7.553	44.494	-7.803	1.00	19.70	B	N



ATOM	3448	CA	GLN	B	41	-7.216	45.914	-7.622	1.00	20.69	B	C
ATOM	3449	CB	GLN	B	41	-8.286	46.641	-6.813	1.00	20.30	B	C
ATOM	3450	CG	GLN	B	41	-8.068	48.173	-6.731	1.00	20.90	B	C
ATOM	3451	CD	GLN	B	41	-8.159	48.842	-8.083	1.00	21.54	B	C
ATOM	3452	OE1	GLN	B	41	-9.070	48.529	-8.858	1.00	23.88	B	O
ATOM	3453	NE2	GLN	B	41	-7.224	49.762	-8.384	1.00	20.95	B	N
ATOM	3454	C	GLN	B	41	-5.880	46.050	-6.906	1.00	22.10	B	C
ATOM	3455	O	GLN	B	41	-5.105	46.941	-7.213	1.00	22.64	B	O
ATOM	3456	N	ASP	B	42	-5.625	45.149	-5.955	1.00	22.70	B	N
ATOM	3457	CA	ASP	B	42	-4.396	45.178	-5.161	1.00	23.28	B	C
ATOM	3458	CB	ASP	B	42	-4.654	44.531	-3.800	1.00	22.77	B	C
ATOM	3459	CG	ASP	B	42	-5.531	45.369	-2.928	1.00	24.12	B	C
ATOM	3460	OD1	ASP	B	42	-5.619	46.599	-3.174	1.00	27.20	B	O
ATOM	3461	OD2	ASP	B	42	-6.206	44.899	-1.991	1.00	25.78	B	O
ATOM	3462	C	ASP	B	42	-3.273	44.438	-5.859	1.00	23.19	B	C
ATOM	3463	O	ASP	B	42	-2.103	44.761	-5.700	1.00	24.27	B	O
ATOM	3464	N	LYS	B	43	-3.629	43.444	-6.655	1.00	22.96	B	N
ATOM	3465	CA	LYS	B	43	-2.634	42.541	-7.203	1.00	23.10	B	C
ATOM	3466	CB	LYS	B	43	-2.508	41.291	-6.299	1.00	23.07	B	C
ATOM	3467	CG	LYS	B	43	-1.376	40.306	-6.701	1.00	23.16	B	C
ATOM	3468	CD	LYS	B	43	-1.348	39.100	-5.750	1.00	24.15	B	C
ATOM	3469	CE	LYS	B	43	-0.391	37.996	-6.217	1.00	25.40	B	C
ATOM	3470	NZ	LYS	B	43	1.031	38.403	-6.170	1.00	25.72	B	N
ATOM	3471	C	LYS	B	43	-3.067	42.157	-8.593	1.00	23.00	B	C
ATOM	3472	O	LYS	B	43	-3.672	41.107	-8.782	1.00	22.17	B	O
ATOM	3473	N	PRO	B	44	-2.772	43.010	-9.571	1.00	24.07	B	N
ATOM	3474	CA	PRO	B	44	-3.282	42.826	-10.948	1.00	24.35	B	C
ATOM	3475	CB	PRO	B	44	-2.632	43.985	-11.735	1.00	24.65	B	C
ATOM	3476	CG	PRO	B	44	-2.197	44.997	-10.702	1.00	25.50	B	C
ATOM	3477	CD	PRO	B	44	-1.960	44.238	-9.415	1.00	24.73	B	C
ATOM	3478	C	PRO	B	44	-2.929	41.486	-11.583	1.00	24.65	B	C
ATOM	3479	O	PRO	B	44	-3.680	40.967	-12.409	1.00	25.49	B	O
ATOM	3480	N	GLU	B	45	-1.778	40.935	-11.206	1.00	25.20	B	N
ATOM	3481	CA	GLU	B	45	-1.310	39.651	-11.725	1.00	25.70	B	C
ATOM	3482	CB	GLU	B	45	0.226	39.599	-11.602	1.00	26.83	B	C
ATOM	3483	CG	GLU	B	45	0.764	39.243	-10.206	1.00	28.74	B	C
ATOM	3484	CD	GLU	B	45	0.925	40.423	-9.262	1.00	32.92	B	C
ATOM	3485	OE1	GLU	B	45	1.667	40.252	-8.253	1.00	34.10	B	O
ATOM	3486	OE2	GLU	B	45	0.316	41.511	-9.488	1.00	33.16	B	O
ATOM	3487	C	GLU	B	45	-1.945	38.404	-11.048	1.00	25.32	B	C
ATOM	3488	O	GLU	B	45	-1.679	37.270	-11.452	1.00	25.52	B	O
ATOM	3489	N	ALA	B	46	-2.788	38.593	-10.034	1.00	24.59	B	N
ATOM	3490	CA	ALA	B	46	-3.327	37.441	-9.309	1.00	23.90	B	C
ATOM	3491	CB	ALA	B	46	-4.271	37.895	-8.229	1.00	23.95	B	C
ATOM	3492	C	ALA	B	46	-4.015	36.426	-10.216	1.00	23.75	B	C
ATOM	3493	O	ALA	B	46	-4.777	36.788	-11.103	1.00	22.67	B	O
ATOM	3494	N	GLN	B	47	-3.717	35.150	-9.982	1.00	23.77	B	N
ATOM	3495	CA	GLN	B	47	-4.438	34.035	-10.568	1.00	24.59	B	C
ATOM	3496	CB	GLN	B	47	-3.479	32.976	-11.105	1.00	25.29	B	C
ATOM	3497	CG	GLN	B	47	-2.425	33.498	-12.080	1.00	28.88	B	C
ATOM	3498	CD	GLN	B	47	-3.025	33.975	-13.393	1.00	35.56	B	C
ATOM	3499	OE1	GLN	B	47	-3.624	33.176	-14.144	1.00	40.01	B	O
ATOM	3500	NE2	GLN	B	47	-2.869	35.278	-13.686	1.00	38.46	B	N
ATOM	3501	C	GLN	B	47	-5.298	33.425	-9.460	1.00	23.84	B	C
ATOM	3502	O	GLN	B	47	-4.786	32.790	-8.517	1.00	24.12	B	O
ATOM	3503	N	ILE	B	48	-6.597	33.644	-9.559	1.00	22.91	B	N
ATOM	3504	CA	ILE	B	48	-7.502	33.329	-8.463	1.00	23.01	B	C
ATOM	3505	CB	ILE	B	48	-8.486	34.462	-8.235	1.00	22.88	B	C



ATOM	3506	CG1	ILE	B	48	-7.708	35.747	-7.988	1.00	22.10	B	C
ATOM	3507	CD1	ILE	B	48	-8.568	36.992	-7.917	1.00	22.38	B	C
ATOM	3508	CG2	ILE	B	48	-9.391	34.161	-7.036	1.00	21.57	B	C
ATOM	3509	C	ILE	B	48	-8.230	32.047	-8.746	1.00	23.69	B	C
ATOM	3510	O	ILE	B	48	-8.685	31.820	-9.877	1.00	23.31	B	O
ATOM	3511	N	ILE	B	49	-8.277	31.206	-7.716	1.00	23.55	B	N
ATOM	3512	CA	ILE	B	49	-8.894	29.894	-7.746	1.00	24.95	B	C
ATOM	3513	CB	ILE	B	49	-7.803	28.812	-7.480	1.00	26.22	B	C
ATOM	3514	CG1	ILE	B	49	-6.723	28.868	-8.575	1.00	29.02	B	C
ATOM	3515	CD1	ILE	B	49	-7.264	28.733	-9.982	1.00	29.18	B	C
ATOM	3516	CG2	ILE	B	49	-8.409	27.422	-7.364	1.00	28.74	B	C
ATOM	3517	C	ILE	B	49	-9.903	29.851	-6.610	1.00	23.74	B	C
ATOM	3518	O	ILE	B	49	-9.620	30.348	-5.511	1.00	24.09	B	O
ATOM	3519	N	VAL	B	50	-11.045	29.224	-6.847	1.00	22.75	B	N
ATOM	3520	CA	VAL	B	50	-12.088	29.110	-5.838	1.00	22.00	B	C
ATOM	3521	CB	VAL	B	50	-13.441	29.682	-6.364	1.00	21.55	B	C
ATOM	3522	CG1	VAL	B	50	-14.583	29.378	-5.388	1.00	22.01	B	C
ATOM	3523	CG2	VAL	B	50	-13.338	31.190	-6.581	1.00	21.04	B	C
ATOM	3524	C	VAL	B	50	-12.273	27.639	-5.439	1.00	21.99	B	C
ATOM	3525	O	VAL	B	50	-12.375	26.780	-6.291	1.00	21.98	B	O
ATOM	3526	N	LEU	B	51	-12.318	27.363	-4.141	1.00	21.70	B	N
ATOM	3527	CA	LEU	B	51	-12.460	26.003	-3.643	1.00	22.26	B	C
ATOM	3528	CB	LEU	B	51	-11.110	25.407	-3.219	1.00	22.70	B	C
ATOM	3529	CG	LEU	B	51	-10.067	25.113	-4.267	1.00	25.11	B	C
ATOM	3530	CD1	LEU	B	51	-8.762	24.764	-3.495	1.00	25.85	B	C
ATOM	3531	CD2	LEU	B	51	-10.513	23.968	-5.183	1.00	27.79	B	C
ATOM	3532	C	LEU	B	51	-13.312	25.997	-2.406	1.00	21.80	B	C
ATOM	3533	O	LEU	B	51	-13.289	26.962	-1.646	1.00	21.46	B	O
ATOM	3534	N	PRO	B	52	-14.006	24.886	-2.163	1.00	21.76	B	N
ATOM	3535	CA	PRO	B	52	-14.750	24.709	-0.921	1.00	22.13	B	C
ATOM	3536	CB	PRO	B	52	-15.340	23.290	-1.071	1.00	23.06	B	C
ATOM	3537	CG	PRO	B	52	-15.389	23.059	-2.525	1.00	22.20	B	C
ATOM	3538	CD	PRO	B	52	-14.145	23.724	-3.058	1.00	22.25	B	C
ATOM	3539	C	PRO	B	52	-13.836	24.809	0.290	1.00	22.83	B	C
ATOM	3540	O	PRO	B	52	-12.682	24.367	0.252	1.00	22.05	B	O
ATOM	3541	N	VAL	B	53	-14.340	25.400	1.365	1.00	23.43	B	N
ATOM	3542	CA	VAL	B	53	-13.579	25.504	2.581	1.00	23.96	B	C
ATOM	3543	CB	VAL	B	53	-14.297	26.368	3.643	1.00	24.41	B	C
ATOM	3544	CG1	VAL	B	53	-15.583	25.692	4.134	1.00	25.13	B	C
ATOM	3545	CG2	VAL	B	53	-13.360	26.671	4.805	1.00	25.93	B	C
ATOM	3546	C	VAL	B	53	-13.324	24.083	3.068	1.00	24.12	B	C
ATOM	3547	O	VAL	B	53	-14.153	23.193	2.859	1.00	24.69	B	O
ATOM	3548	N	GLY	B	54	-12.158	23.867	3.657	1.00	22.87	B	N
ATOM	3549	CA	GLY	B	54	-11.765	22.548	4.117	1.00	22.48	B	C
ATOM	3550	C	GLY	B	54	-11.067	21.662	3.092	1.00	21.22	B	C
ATOM	3551	O	GLY	B	54	-10.597	20.606	3.453	1.00	21.63	B	O
ATOM	3552	N	THR	B	55	-10.977	22.091	1.837	1.00	20.24	B	N
ATOM	3553	CA	THR	B	55	-10.295	21.324	0.809	1.00	19.46	B	C
ATOM	3554	CB	THR	B	55	-10.469	22.006	-0.573	1.00	19.86	B	C
ATOM	3555	OG1	THR	B	55	-11.866	22.158	-0.875	1.00	22.41	B	O
ATOM	3556	CG2	THR	B	55	-9.957	21.139	-1.701	1.00	19.94	B	C
ATOM	3557	C	THR	B	55	-8.788	21.125	1.077	1.00	17.93	B	C
ATOM	3558	O	THR	B	55	-8.057	22.042	1.417	1.00	16.91	B	O
ATOM	3559	N	ILE	B	56	-8.336	19.911	0.849	1.00	17.04	B	N
ATOM	3560	CA	ILE	B	56	-6.929	19.571	0.943	1.00	16.44	B	C
ATOM	3561	CB	ILE	B	56	-6.800	18.076	1.232	1.00	15.71	B	C
ATOM	3562	CG1	ILE	B	56	-7.439	17.782	2.600	1.00	17.41	B	C
ATOM	3563	CD1	ILE	B	56	-7.353	16.319	3.098	1.00	17.17	B	C

ATOM	3564	CG2	ILE	B	56	-5.347	17.684	1.247	1.00	16.77	B	C
ATOM	3565	C	ILE	B	56	-6.217	19.981	-0.336	1.00	16.51	B	C
ATOM	3566	O	ILE	B	56	-6.701	19.691	-1.434	1.00	17.03	B	O
ATOM	3567	N	VAL	B	57	-5.088	20.678	-0.203	1.00	15.94	B	N
ATOM	3568	CA	VAL	B	57	-4.342	21.200	-1.361	1.00	16.45	B	C
ATOM	3569	CB	VAL	B	57	-4.511	22.726	-1.488	1.00	16.21	B	C
ATOM	3570	CG1	VAL	B	57	-6.012	23.092	-1.672	1.00	16.73	B	C
ATOM	3571	CG2	VAL	B	57	-3.991	23.435	-0.236	1.00	18.16	B	C
ATOM	3572	C	VAL	B	57	-2.853	20.910	-1.205	1.00	16.63	B	C
ATOM	3573	O	VAL	B	57	-2.393	20.624	-0.099	1.00	16.42	B	O
ATOM	3574	N	THR	B	58	-2.106	20.982	-2.299	1.00	17.06	B	N
ATOM	3575	CA	THR	B	58	-0.658	20.801	-2.247	1.00	16.63	B	C
ATOM	3576	CB	THR	B	58	-0.069	20.712	-3.654	1.00	17.18	B	C
ATOM	3577	OG1	THR	B	58	-0.660	21.718	-4.494	1.00	15.16	B	O
ATOM	3578	CG2	THR	B	58	-0.423	19.426	-4.292	1.00	19.58	B	C
ATOM	3579	C	THR	B	58	-0.093	22.017	-1.536	1.00	16.72	B	C
ATOM	3580	O	THR	B	58	-0.756	23.071	-1.492	1.00	16.30	B	O
ATOM	3581	N	MET	B	59	1.103	21.885	-0.960	1.00	16.38	B	N
ATOM	3582	CA	MET	B	59	1.692	22.982	-0.180	1.00	16.07	B	C
ATOM	3583	CB	MET	B	59	1.960	22.552	1.254	1.00	15.92	B	C
ATOM	3584	CG	MET	B	59	0.668	22.365	2.012	1.00	16.14	B	C
ATOM	3585	SD	MET	B	59	-0.197	23.961	2.251	1.00	17.09	B	S
ATOM	3586	CE	MET	B	59	-1.612	23.424	3.218	1.00	17.23	B	C
ATOM	3587	C	MET	B	59	2.911	23.607	-0.816	1.00	15.83	B	C
ATOM	3588	O	MET	B	59	3.884	23.983	-0.134	1.00	15.99	B	O
ATOM	3589	N	GLU	B	60	2.837	23.794	-2.127	1.00	15.11	B	N
ATOM	3590	CA	GLU	B	60	3.838	24.609	-2.795	1.00	15.22	B	C
ATOM	3591	CB	GLU	B	60	4.155	24.079	-4.187	1.00	15.39	B	C
ATOM	3592	CG	GLU	B	60	3.299	24.609	-5.334	1.00	15.29	B	C
ATOM	3593	CD	GLU	B	60	1.845	24.166	-5.270	1.00	19.22	B	C
ATOM	3594	OE1	GLU	B	60	1.435	23.486	-4.308	1.00	18.05	B	O
ATOM	3595	OE2	GLU	B	60	1.087	24.526	-6.195	1.00	18.12	B	O
ATOM	3596	C	GLU	B	60	3.344	26.081	-2.771	1.00	15.50	B	C
ATOM	3597	O	GLU	B	60	2.133	26.356	-2.798	1.00	15.17	B	O
ATOM	3598	N	TYR	B	61	4.292	27.011	-2.721	1.00	16.00	B	N
ATOM	3599	CA	TYR	B	61	3.982	28.431	-2.654	1.00	17.37	B	C
ATOM	3600	CB	TYR	B	61	4.938	29.138	-1.699	1.00	17.67	B	C
ATOM	3601	CG	TYR	B	61	4.671	30.623	-1.493	1.00	18.81	B	C
ATOM	3602	CD1	TYR	B	61	5.474	31.572	-2.103	1.00	21.63	B	C
ATOM	3603	CE1	TYR	B	61	5.233	32.895	-1.943	1.00	21.96	B	C
ATOM	3604	CZ	TYR	B	61	4.207	33.299	-1.134	1.00	22.89	B	C
ATOM	3605	OH	TYR	B	61	4.007	34.644	-0.972	1.00	29.91	B	O
ATOM	3606	CE2	TYR	B	61	3.407	32.394	-0.507	1.00	20.81	B	C
ATOM	3607	CD2	TYR	B	61	3.637	31.059	-0.697	1.00	19.36	B	C
ATOM	3608	C	TYR	B	61	4.067	29.037	-4.048	1.00	18.22	B	C
ATOM	3609	O	TYR	B	61	5.126	29.041	-4.654	1.00	18.04	B	O
ATOM	3610	N	ARG	B	62	2.943	29.531	-4.564	1.00	19.75	B	N
ATOM	3611	CA	ARG	B	62	2.938	30.226	-5.861	1.00	21.16	B	C
ATOM	3612	CB	ARG	B	62	1.909	29.625	-6.814	1.00	21.92	B	C
ATOM	3613	CG	ARG	B	62	2.189	28.185	-7.196	1.00	25.65	B	C
ATOM	3614	CD	ARG	B	62	1.385	27.694	-8.421	1.00	29.39	B	C
ATOM	3615	NE	ARG	B	62	1.516	26.235	-8.639	1.00	32.04	B	N
ATOM	3616	CZ	ARG	B	62	0.982	25.593	-9.675	1.00	33.94	B	C
ATOM	3617	NH1	ARG	B	62	1.129	24.287	-9.798	1.00	37.42	B	N
ATOM	3618	NH2	ARG	B	62	0.292	26.255	-10.586	1.00	34.66	B	N
ATOM	3619	C	ARG	B	62	2.619	31.687	-5.652	1.00	21.86	B	C
ATOM	3620	O	ARG	B	62	1.491	32.033	-5.296	1.00	21.34	B	O
ATOM	3621	N	ILE	B	63	3.609	32.547	-5.894	1.00	23.01	B	N

ATOM	3622	CA	ILE	B	63	3.503	33.950	-5.502	1.00	24.71	B	C
ATOM	3623	CB	ILE	B	63	4.824	34.707	-5.709	1.00	25.05	B	C
ATOM	3624	CG1	ILE	B	63	4.790	36.033	-4.919	1.00	28.83	B	C
ATOM	3625	CD1	ILE	B	63	6.158	36.609	-4.546	1.00	31.61	B	C
ATOM	3626	CG2	ILE	B	63	5.047	34.966	-7.207	1.00	26.58	B	C
ATOM	3627	C	ILE	B	63	2.367	34.699	-6.216	1.00	24.34	B	C
ATOM	3628	O	ILE	B	63	1.860	35.675	-5.672	1.00	25.45	B	O
ATOM	3629	N	ASP	B	64	1.961	34.240	-7.398	1.00	24.15	B	N
ATOM	3630	CA	ASP	B	64	0.901	34.919	-8.153	1.00	24.63	B	C
ATOM	3631	CB	BASP	B	64	1.214	34.889	-9.664	0.40	24.94	B	C
ATOM	3632	CB	AASP	B	64	1.201	34.873	-9.650	0.60	24.96	B	C
ATOM	3633	CG	BASP	B	64	0.987	33.514	-10.307	0.40	25.65	B	C
ATOM	3634	CG	AASP	B	64	2.403	35.712	-10.026	0.60	25.91	B	C
ATOM	3635	OD1	BASP	B	64	0.745	33.465	-11.536	0.40	27.17	B	O
ATOM	3636	OD1	AASP	B	64	3.136	35.290	-10.950	0.60	27.52	B	O
ATOM	3637	OD2	BASP	B	64	1.054	32.426	-9.686	0.40	28.49	B	O
ATOM	3638	OD2	AASP	B	64	2.704	36.782	-9.439	0.60	26.67	B	O
ATOM	3639	C	ASP	B	64	-0.514	34.361	-7.896	1.00	24.47	B	C
ATOM	3640	O	ASP	B	64	-1.515	34.928	-8.392	1.00	24.83	B	O
ATOM	3641	N	ARG	B	65	-0.601	33.269	-7.136	1.00	21.92	B	N
ATOM	3642	CA	ARG	B	65	-1.876	32.615	-6.893	1.00	21.12	B	C
ATOM	3643	CB	ARG	B	65	-1.677	31.101	-6.737	1.00	19.95	B	C
ATOM	3644	CG	ARG	B	65	-2.946	30.305	-6.463	1.00	18.99	B	C
ATOM	3645	CD	ARG	B	65	-2.730	28.808	-6.572	1.00	19.09	B	C
ATOM	3646	NE	ARG	B	65	-1.784	28.369	-5.554	1.00	18.66	B	N
ATOM	3647	CZ	ARG	B	65	-1.130	27.214	-5.534	1.00	19.41	B	C
ATOM	3648	NH1	ARG	B	65	-1.279	26.300	-6.470	1.00	19.74	B	N
ATOM	3649	NH2	ARG	B	65	-0.311	26.963	-4.522	1.00	21.82	B	N
ATOM	3650	C	ARG	B	65	-2.556	33.168	-5.662	1.00	20.36	B	C
ATOM	3651	O	ARG	B	65	-1.896	33.515	-4.682	1.00	21.06	B	O
ATOM	3652	N	VAL	B	66	-3.875	33.284	-5.727	1.00	20.04	B	N
ATOM	3653	CA	VAL	B	66	-4.692	33.540	-4.560	1.00	19.79	B	C
ATOM	3654	CB	VAL	B	66	-5.266	34.962	-4.510	1.00	19.88	B	C
ATOM	3655	CG1	VAL	B	66	-6.036	35.160	-3.204	1.00	21.06	B	C
ATOM	3656	CG2	VAL	B	66	-4.194	36.004	-4.607	1.00	20.96	B	C
ATOM	3657	C	VAL	B	66	-5.846	32.525	-4.551	1.00	20.19	B	C
ATOM	3658	O	VAL	B	66	-6.733	32.512	-5.444	1.00	20.12	B	O
ATOM	3659	N	ARG	B	67	-5.832	31.654	-3.557	1.00	20.01	B	N
ATOM	3660	CA	ARG	B	67	-6.916	30.713	-3.394	1.00	20.45	B	C
ATOM	3661	CB	ARG	B	67	-6.416	29.437	-2.740	1.00	20.71	B	C
ATOM	3662	CG	ARG	B	67	-5.572	28.538	-3.626	1.00	21.28	B	C
ATOM	3663	CD	ARG	B	67	-5.471	27.144	-3.016	1.00	23.63	B	C
ATOM	3664	NE	ARG	B	67	-4.539	26.204	-3.632	1.00	22.50	B	N
ATOM	3665	CZ	ARG	B	67	-3.326	25.921	-3.160	1.00	24.19	B	C
ATOM	3666	NH1	ARG	B	67	-2.589	24.992	-3.759	1.00	22.65	B	N
ATOM	3667	NH2	ARG	B	67	-2.837	26.571	-2.106	1.00	22.06	B	N
ATOM	3668	C	ARG	B	67	-8.001	31.368	-2.543	1.00	20.49	B	C
ATOM	3669	O	ARG	B	67	-7.704	31.990	-1.529	1.00	20.17	B	O
ATOM	3670	N	LEU	B	68	-9.255	31.253	-2.970	1.00	20.39	B	N
ATOM	3671	CA	LEU	B	68	-10.373	31.705	-2.148	1.00	21.05	B	C
ATOM	3672	CB	LEU	B	68	-11.323	32.604	-2.957	1.00	21.11	B	C
ATOM	3673	CG	LEU	B	68	-10.701	33.830	-3.627	1.00	21.59	B	C
ATOM	3674	CD1	LEU	B	68	-11.745	34.523	-4.508	1.00	22.82	B	C
ATOM	3675	CD2	LEU	B	68	-10.187	34.785	-2.595	1.00	22.44	B	C
ATOM	3676	C	LEU	B	68	-11.132	30.493	-1.648	1.00	21.12	B	C
ATOM	3677	O	LEU	B	68	-11.663	29.709	-2.432	1.00	21.87	B	O
ATOM	3678	N	PHE	B	69	-11.209	30.345	-0.345	1.00	21.61	B	N
ATOM	3679	CA	PHE	B	69	-11.937	29.226	0.233	1.00	21.97	B	C

ATOM	3680	CB	PHE	B	69	-11.151	28.647	1.422	1.00	22.17	B	C
ATOM	3681	CG	PHE	B	69	-9.896	27.905	1.028	1.00	19.89	B	C
ATOM	3682	CD1	PHE	B	69	-9.938	26.557	0.737	1.00	21.41	B	C
ATOM	3683	CE1	PHE	B	69	-8.788	25.862	0.370	1.00	20.29	B	C
ATOM	3684	CZ	PHE	B	69	-7.598	26.525	0.290	1.00	21.78	B	C
ATOM	3685	CE2	PHE	B	69	-7.542	27.879	0.575	1.00	21.52	B	C
ATOM	3686	CD2	PHE	B	69	-8.691	28.557	0.950	1.00	19.33	B	C
ATOM	3687	C	PHE	B	69	-13.321	29.725	0.664	1.00	23.11	B	C
ATOM	3688	O	PHE	B	69	-13.414	30.651	1.506	1.00	22.87	B	O
ATOM	3689	N	VAL	B	70	-14.371	29.105	0.111	1.00	24.00	B	N
ATOM	3690	CA	VAL	B	70	-15.755	29.578	0.289	1.00	25.82	B	C
ATOM	3691	CB	VAL	B	70	-16.442	29.958	-1.054	1.00	25.72	B	C
ATOM	3692	CG1	VAL	B	70	-15.686	31.063	-1.756	1.00	26.70	B	C
ATOM	3693	CG2	VAL	B	70	-16.599	28.756	-1.958	1.00	26.63	B	C
ATOM	3694	C	VAL	B	70	-16.691	28.602	0.996	1.00	26.63	B	C
ATOM	3695	O	VAL	B	70	-16.532	27.380	0.899	1.00	27.14	B	O
ATOM	3696	N	ASP	B	71	-17.664	29.155	1.714	1.00	27.52	B	N
ATOM	3697	CA	ASP	B	71	-18.686	28.352	2.399	1.00	29.00	B	C
ATOM	3698	CB	ASP	B	71	-19.247	29.132	3.591	1.00	28.91	B	C
ATOM	3699	CG	ASP	B	71	-20.019	30.392	3.171	1.00	28.74	B	C
ATOM	3700	OD1	ASP	B	71	-20.161	31.290	4.018	1.00	29.94	B	O
ATOM	3701	OD2	ASP	B	71	-20.509	30.572	2.032	1.00	27.69	B	O
ATOM	3702	C	ASP	B	71	-19.796	27.931	1.413	1.00	30.37	B	C
ATOM	3703	O	ASP	B	71	-19.646	28.098	0.217	1.00	29.90	B	O
ATOM	3704	N	LYS	B	72	-20.898	27.376	1.906	1.00	33.42	B	N
ATOM	3705	CA	LYS	B	72	-21.949	26.822	1.022	1.00	34.98	B	C
ATOM	3706	CB	LYS	B	72	-22.951	26.004	1.834	1.00	35.44	B	C
ATOM	3707	CG	LYS	B	72	-22.190	24.925	2.916	0.00	40.00	B	C
ATOM	3708	CD	LYS	B	72	-22.489	23.435	2.595	0.00	40.00	B	C
ATOM	3709	CE	LYS	B	72	-21.240	22.528	2.667	0.00	40.00	B	C
ATOM	3710	NZ	LYS	B	72	-21.120	21.662	1.456	0.00	40.00	B	N
ATOM	3711	C	LYS	B	72	-22.709	27.904	0.261	1.00	36.38	B	C
ATOM	3712	O	LYS	B	72	-23.332	27.627	-0.766	1.00	37.77	B	O
ATOM	3713	N	LEU	B	73	-22.640	29.138	0.753	1.00	37.07	B	N
ATOM	3714	CA	LEU	B	73	-23.306	30.286	0.114	1.00	37.22	B	C
ATOM	3715	CB	LEU	B	73	-23.759	31.265	1.201	1.00	37.50	B	C
ATOM	3716	CG	LEU	B	73	-24.711	30.678	2.254	1.00	40.20	B	C
ATOM	3717	CD1	LEU	B	73	-25.387	31.796	3.053	1.00	41.53	B	C
ATOM	3718	CD2	LEU	B	73	-25.782	29.775	1.612	1.00	41.89	B	C
ATOM	3719	C	LEU	B	73	-22.406	31.008	-0.890	1.00	36.59	B	C
ATOM	3720	O	LEU	B	73	-22.781	32.029	-1.482	1.00	36.18	B	O
ATOM	3721	N	ASP	B	74	-21.203	30.468	-1.076	1.00	36.33	B	N
ATOM	3722	CA	ASP	B	74	-20.192	31.084	-1.923	1.00	35.65	B	C
ATOM	3723	CB	ASP	B	74	-20.709	31.252	-3.342	1.00	36.81	B	C
ATOM	3724	CG	ASP	B	74	-20.063	30.283	-4.286	1.00	40.36	B	C
ATOM	3725	OD1	ASP	B	74	-19.429	30.756	-5.259	1.00	45.75	B	O
ATOM	3726	OD2	ASP	B	74	-20.108	29.032	-4.101	1.00	45.61	B	O
ATOM	3727	C	ASP	B	74	-19.646	32.399	-1.381	1.00	33.94	B	C
ATOM	3728	O	ASP	B	74	-19.147	33.249	-2.136	1.00	34.59	B	O
ATOM	3729	N	ASN	B	75	-19.696	32.546	-0.066	1.00	31.85	B	N
ATOM	3730	CA	ASN	B	75	-19.000	33.634	0.597	1.00	30.66	B	C
ATOM	3731	CB	ASN	B	75	-19.877	34.185	1.714	1.00	30.45	B	C
ATOM	3732	CG	ASN	B	75	-21.170	34.793	1.176	1.00	30.77	B	C
ATOM	3733	OD1	ASN	B	75	-21.169	35.401	0.102	1.00	30.57	B	O
ATOM	3734	ND2	ASN	B	75	-22.275	34.615	1.907	1.00	30.32	B	N
ATOM	3735	C	ASN	B	75	-17.628	33.213	1.127	1.00	29.26	B	C
ATOM	3736	O	ASN	B	75	-17.433	32.073	1.553	1.00	29.07	B	O
ATOM	3737	N	ILE	B	76	-16.685	34.143	1.086	1.00	27.83	B	N



ATOM	3738	CA	ILE	B	76	-15.337	33.893	1.540	1.00	26.88	B	C
ATOM	3739	CB	ILE	B	76	-14.511	35.182	1.455	1.00	26.51	B	C
ATOM	3740	CG1	ILE	B	76	-14.474	35.737	0.020	1.00	26.61	B	C
ATOM	3741	CD1	ILE	B	76	-14.130	34.728	-1.039	1.00	26.87	B	C
ATOM	3742	CG2	ILE	B	76	-13.137	34.927	1.993	1.00	25.62	B	C
ATOM	3743	C	ILE	B	76	-15.401	33.382	2.993	1.00	26.59	B	C
ATOM	3744	O	ILE	B	76	-15.994	34.017	3.838	1.00	26.12	B	O
ATOM	3745	N	ALA	B	77	-14.795	32.237	3.263	1.00	26.58	B	N
ATOM	3746	CA	ALA	B	77	-14.899	31.582	4.576	1.00	26.79	B	C
ATOM	3747	CB	ALA	B	77	-15.129	30.088	4.386	1.00	26.56	B	C
ATOM	3748	C	ALA	B	77	-13.670	31.815	5.467	1.00	26.89	B	C
ATOM	3749	O	ALA	B	77	-13.764	31.751	6.677	1.00	27.73	B	O
ATOM	3750	N	GLU	B	78	-12.518	32.072	4.871	1.00	26.32	B	N
ATOM	3751	CA	GLU	B	78	-11.355	32.446	5.647	1.00	26.33	B	C
ATOM	3752	CB	GLU	B	78	-10.508	31.216	6.041	1.00	26.80	B	C
ATOM	3753	CG	GLU	B	78	-10.106	30.290	4.921	1.00	27.82	B	C
ATOM	3754	CD	GLU	B	78	-9.956	28.827	5.352	1.00	28.92	B	C
ATOM	3755	OE1	GLU	B	78	-9.785	28.493	6.559	1.00	36.40	B	O
ATOM	3756	OE2	GLU	B	78	-10.001	27.977	4.472	1.00	28.50	B	O
ATOM	3757	C	GLU	B	78	-10.530	33.478	4.895	1.00	25.94	B	C
ATOM	3758	O	GLU	B	78	-10.807	33.805	3.712	1.00	25.71	B	O
ATOM	3759	N	VAL	B	79	-9.527	33.996	5.594	1.00	24.85	B	N
ATOM	3760	CA	VAL	B	79	-8.712	35.088	5.102	1.00	24.88	B	C
ATOM	3761	CB	VAL	B	79	-7.692	35.578	6.167	1.00	25.77	B	C
ATOM	3762	CG1	VAL	B	79	-6.814	36.672	5.583	1.00	25.38	B	C
ATOM	3763	CG2	VAL	B	79	-8.396	36.073	7.456	1.00	26.10	B	C
ATOM	3764	C	VAL	B	79	-7.957	34.652	3.835	1.00	24.07	B	C
ATOM	3765	O	VAL	B	79	-7.137	33.742	3.883	1.00	23.32	B	O
ATOM	3766	N	PRO	B	80	-8.275	35.271	2.699	1.00	23.27	B	N
ATOM	3767	CA	PRO	B	80	-7.533	35.029	1.466	1.00	22.93	B	C
ATOM	3768	CB	PRO	B	80	-8.296	35.856	0.426	1.00	23.15	B	C
ATOM	3769	CG	PRO	B	80	-9.645	36.042	1.005	1.00	23.83	B	C
ATOM	3770	CD	PRO	B	80	-9.404	36.194	2.480	1.00	23.67	B	C
ATOM	3771	C	PRO	B	80	-6.101	35.512	1.601	1.00	22.05	B	C
ATOM	3772	O	PRO	B	80	-5.891	36.588	2.136	1.00	20.76	B	O
ATOM	3773	N	ARG	B	81	-5.147	34.691	1.190	1.00	21.54	B	N
ATOM	3774	CA	ARG	B	81	-3.765	35.135	1.074	1.00	22.93	B	C
ATOM	3775	CB	BARG	B	81	-2.937	34.683	2.298	0.40	22.99	B	C
ATOM	3776	CB	AARG	B	81	-2.865	34.764	2.275	0.60	23.27	B	C
ATOM	3777	CG	BARG	B	81	-3.684	34.672	3.645	0.40	24.27	B	C
ATOM	3778	CG	AARG	B	81	-3.278	33.619	3.175	0.60	25.79	B	C
ATOM	3779	CD	BARG	B	81	-2.996	33.818	4.744	0.40	26.79	B	C
ATOM	3780	CD	AARG	B	81	-2.615	33.723	4.575	0.60	27.67	B	C
ATOM	3781	NE	BARG	B	81	-3.975	33.234	5.664	0.40	28.96	B	N
ATOM	3782	NE	AARG	B	81	-3.283	32.907	5.581	0.60	29.38	B	N
ATOM	3783	CZ	BARG	B	81	-4.567	32.053	5.508	0.40	29.28	B	C
ATOM	3784	CZ	AARG	B	81	-3.934	33.381	6.642	0.60	30.17	B	C
ATOM	3785	NH1	BARG	B	81	-4.284	31.274	4.471	0.40	31.06	B	N
ATOM	3786	NH1	AARG	B	81	-4.020	34.680	6.867	0.60	31.08	B	N
ATOM	3787	NH2	BARG	B	81	-5.448	31.645	6.408	0.40	30.62	B	N
ATOM	3788	NH2	AARG	B	81	-4.510	32.545	7.486	0.60	31.16	B	N
ATOM	3789	C	ARG	B	81	-3.115	34.616	-0.178	1.00	21.97	B	C
ATOM	3790	O	ARG	B	81	-3.560	33.632	-0.761	1.00	21.68	B	O
ATOM	3791	N	VAL	B	82	-2.029	35.286	-0.559	1.00	20.91	B	N
ATOM	3792	CA	VAL	B	82	-1.224	34.884	-1.679	1.00	21.03	B	C
ATOM	3793	CB	VAL	B	82	-0.126	35.943	-1.952	1.00	21.89	B	C
ATOM	3794	CG1	VAL	B	82	0.869	35.435	-2.906	1.00	22.93	B	C
ATOM	3795	CG2	VAL	B	82	-0.734	37.243	-2.483	1.00	21.44	B	C



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ATOM	3796	C	VAL	B	82	-0.583	33.532	-1.371	1.00	20.69	B	C
ATOM	3797	O	VAL	B	82	-0.235	33.255	-0.221	1.00	19.36	B	O
ATOM	3798	N	GLY	B	83	-0.469	32.694	-2.389	1.00	19.91	B	N
ATOM	3799	CA	GLY	B	83	0.382	31.525	-2.331	1.00	20.16	B	C
ATOM	3800	C	GLY	B	83	-0.236	30.295	-2.955	1.00	20.11	B	C
ATOM	3801	O	GLY	B	83	-1.416	30.328	-3.319	1.00	20.36	B	O
ATOM	3802	OXT	GLY	B	83	0.468	29.294	-3.104	1.00	18.79	B	O